Fast numerical solution of nonlinear diffusion equation for the simulation of ion-exchanged micro-optics components in glass

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Modulation of the refractive index of glass using ion exchange is a common fabrication method for various micro-optics components, such as waveguide devices, microlenses, and diffractive elements. The design of elements with complicated optical functions has increased the demand for fast numerical simulation of the nonlinear ion-exchange process of two monovalent ions. In this paper, a linear implicit finite-difference Crank-Nicholson-type method is implemented for thermal two- and three-dimensional ion-exchange processes. The resulting system of linear equations is solved by using various iterative methods. Grid spacing, length of the time step, and the number of iterations are chosen so that desired accuracy is obtained within minimum computing time. The implemented methods are compared with the Peaceman-Rachford Alternating Direction Implicit (PR–ADI) and the explicit Du Fort–Frankel method in modeling a computer-synthesized diffractive optical element and a waveguide channel system.

Key words: ion exchange in glass, gradient-index, numerical simulation
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1 Introduction

Ion exchange in glass is a major candidate for the fabrication of passive components used in fiber-optic telecommunication, such as splitters and wavelength division multiplexers [1–3]. The local variation of the refractive index in glass has also been utilized in microlenses [4–6]. Recently, we proposed and demonstrated the fabrication of graded-index computer-synthesized diffractive optical elements (DOEs) with high diffraction efficiency using thermal ion exchange [7,8].

Besides a rigid structure of so-called glass-formers, glass also contains minor proportions of so-called network modifiers, such as K_2O, which mainly have effects on glass properties, such as hardness and refractive index [9]. If a glass substrate is immersed in a salt melt at a temperature well below the melting point of the glass, the metal ions of the modifiers (denoted by A) are free to move and to be exchanged with other metal ions, e.g., Ag^+, in the salt melt (denoted by B). The physical phenomena responsible for the exchange process are diffusion and convection. Refractive index modulation is caused by three major physical changes: ionic polarizability, molar volume, and stresses created by the exchange of ions with different radii. The ion-exchange process in a glass substrate can be spatially controlled using a patterned mask with apertures.

The nonlinear diffusion equation describing the thermal ion exchange of two monovalent ions in glass is given as [10]

$$\frac{\partial C}{\partial t} = \nabla \cdot \left[\frac{D_A \nabla C}{(M-1)C+1}\right] = \frac{D_A \nabla^2 C}{C(M-1)+1} - \frac{D_A (M-1) \nabla C \cdot \nabla C}{[C(M-1)+1]^2}. \quad (1)$$

The concentration has been normalized to the interval 0...1 by $C = C_A/C_0$, where $C_0 = C_A + C_B = \text{const.}$, and C_A and C_B are the concentrations of the ions A and B in the glass, respectively. In case of field-assisted ion exchange Eq. (1) has an additional convection term. D_A is the self-diffusion constant of the ions A and $M = D_A/D_B$ is the ratio of the self-diffusion constants of the ions A and B. Nonlinearity in Eq. (1) disappears when $M = 1$, and then Eq. (1) reduces to the linear diffusion equation

$$\frac{\partial C}{\partial t} = D_A \nabla^2 C. \quad (2)$$

The boundary conditions are $C = 1$ at the surface under apertures and $\partial C/\partial y = 0$ at the surface under mask, where y axis is perpendicular to the surface. In the case of a periodic mask structure with the period of d_x and d_z in x and z direction, respectively, it is enough to analyze only the area of one period: the boundary conditions are $C(0, y, z) = C(d_x, y, z)$ and $C(x, y, 0) = C(x, y, d_z)$. In the case of a grating symmetric in both x and z directions, modeling is needed only in one quarter of the domain with the boundary conditions: $\partial C(0, y, z)/\partial x = 0$, $\partial C(d_x/2, y, z)/\partial x = 0$, $\partial C(x, y, 0)/\partial z = 0$, and $\partial C(x, y, d_z/2)/\partial z = 0$. In two-dimensional ion exchange processes, the mask structure is constant in z direction and C is only a function of x and y coordinates.

Sophisticated design of ion-exchanged waveguide components as well as DOEs with complicated optical functions requires optimization algorithms and simulating the ion exchange process hundreds or thousands of times with different mask configurations. The computation of the refractive index distribution in the glass is much more time consuming than the determination of the optical function, since the diffusion evolves with time. Therefore, a fast solution method of the diffusion equation is required. In this paper, we describe the implementation of an implicit Crank-Nicholson-type finite difference method for solution of the ion-exchange equation. Although implicit finite difference algorithms are widely used even in determining the optical function of channel waveguides by beam-propagation methods [11], they have been regarded as computationally too slow in ion-exchange modeling [12].

For solving the resulting system of linear equations, comparisons of the computing times are made for four different iteration techniques: Successive Over Relaxation (SOR), Conjugate-Gradient (CG), Conjugate-Gradient Squared (CGS), and Quasi Minimal Residual (QMR) method. Further saving in computation time is gained by adaptive time step and grid spacing. As an example, a computer-synthesized DOE for beam splitting and a 2×2 adiabatic 3-dB coupler are analyzed using a Crank-Nicholson-type method, and the results and the computing times are compared with the Peaceman-Rachford Alternating Direction Implicit (PR–ADI) method and the explicit Du Fort–Frankel method.

2 Implementation of implicit finite difference algorithms

In finite difference methods, the solution domain is discretized and the computation nodes form a grid that is rectangular but does not have to be uniform in space or stationary in time. In this work, we use a stationary grid that is uniform in x and z directions, i.e., in planes parallel to the glass surface, and non-uniform in y direction. For discretization in space domain, we use the second-order finite difference schemes for the derivatives ∇C and $\nabla^2 C$, which can be derived using Lagrangian interpolation [13]. For instance,

$$\frac{\partial C_j}{\partial y} \simeq -C_{j-1}\left[\left(\frac{\Delta y_{j+1}}{\Delta y_j}\right)(\Delta y_j + \Delta y_{j+1})^{-1}\right] + C_j\left[(\Delta y_j)^{-1} - (\Delta y_{j+1})^{-1}\right]$$

$$+C_{j+1}\left[\left(\frac{\Delta y_j}{\Delta y_{j+1}}\right)(\Delta y_j + \Delta y_{j+1})^{-1}\right] = \mathcal{A}_y C_{j-1} + \mathcal{B}_y C_j + \mathcal{C}_y C_{j+1}, \quad (3)$$

$$\frac{\partial^2 C_j}{\partial y^2} \simeq 2[\Delta y_j(\Delta y_j + \Delta y_{j+1})]^{-1} C_{j-1} - \frac{2}{\Delta y_j \Delta y_{j+1}} C_j$$

$$+2[\Delta y_{j+1}(\Delta y_j + \Delta y_{j+1})]^{-1} C_{j+1} = \mathcal{D}_y C_{j-1} + \mathcal{E}_y C_j + \mathcal{F}_y C_{j+1}, \quad (4)$$

where $\Delta y_j = y_j - y_{j-1}$ ja $\Delta y_{j+1} = y_{j+1} - y_j$ are the spacing of the nodes in y direction and $\mathcal{A}, \mathcal{B}, ..., \mathcal{F}$ are time-independent, as the grid is stationary. An additional layer of nodes, i.e., C_0, is situated on top of the glass surface, i.e., C_1. The central difference approximation $C_0 = C_2$ is used to implement the zero-flux boundary conditions [13]. The distance between adjacent grid points in x and z direction depends on the desired accuracy of the mask patterning, while in y direction it depends on the ion-exchange process itself. The concentrations at the nodes are treated as a vector $\mathbf{C}$, whose elements are the values of the nodes. The refractive index modulation is be assumed to be linearly dependent on C

$$\Delta n \approx C \Delta n_{\max}, \quad (5)$$

where $\Delta n_{\max}$ is the maximum refractive index change corresponding to $C = 1$.

Denoting the discretized righthandside of Eq. (1) by $\mathcal{L}C$, the second-order Crank-Nicholson method for discretization in time domain reads

$$\frac{C^{l+1} - C^l}{\Delta t} = \mathcal{L}\left(\frac{C^l + C^{l+1}}{2}\right), \quad (6)$$

where l is the index referring to the time step and Δt is the length of the time step. The set of Eqs. (6) is nonlinear and laborious to solve by, e.g. the Newton type methods. Thus, we use the linearly implicit Rosenbrock method [14]

$$\mathbf{k} = \mathcal{L}(\mathbf{C}^l) + \frac{\Delta t}{2}\mathbf{J}\mathbf{k}, \quad (7)$$

$$\mathbf{C}^{l+1} = \mathbf{C}^l + \mathbf{k}\Delta t. \quad (8)$$

The method has stability and accuracy similar to the Crank-Nicholson method, to which it reduces if $M = 1$, as the nonlinearity vanishes. The matrix $\mathbf{J}$ is the Jacobian of $\mathcal{L}\mathbf{C}^l$. Now the problem is reduced to computing $\mathbf{J}$ and solving a linear system of equations

$$\mathbf{A}\mathbf{k} = \mathbf{b}, \tag{9}$$

where $\mathbf{b} = \mathcal{L}(\mathbf{C}^l)$ and $\mathbf{A} = \mathbf{I} - (\Delta t/2)\mathbf{J}$; $\mathbf{I}$ being the unit matrix. In two-dimensional diffusion problem, $\mathbf{A}$ is generally a pentadiagonal, asymmetric matrix. The asymmetry arises from the nonlinear term involving M in Eq. (1). In three-dimensional case, $\mathbf{A}$ consists of seven diagonals.

Several algorithms exist for solving the system of equations resulting from implicit finite difference discretization. In this case, non-iterative solution by, e.g., Gaussian elimination [15] is not efficient enough. For the iterative solution we use the successive over-relaxation (SOR) method with classical red-black ordering of the grid nodes and adaptive determination of the relaxation parameter [16]. Furthermore, we also implement incomplete LU (ILU) preconditioned conjugate-gradient (CG), conjugate-gradient squared (CGS), and the Quasi Minimal Residual (QMR) methods [15,17,18]. The CG is suitable for symmetric, positive-definite matrices, but in our experience, it also works well for solving Eq. (9) even with small values of M in Eq. (1). However, if $M \ll 1$, the CGS and QMR methods seem to be more suitable, as they are generalizations of the CG method for nonsymmetric systems of equations. Both methods are very efficient, but the QMR method is usually considered more stable than the CGS method. In simulation of field-assisted ion exchange, the convection term breaks the symmetry effectively, and the CG method is unlikely to work well.

The sufficient amount of iterations is determined according to a condition that the residual error is of the same order as the error due to the discretization in time. The performance of each iteration method further depends on computer architecture to be used. For instance, the SOR method can be easily implemented in vector computers, but using ILU–preconditioning in the Conjugate Gradient type methods usually demands a special implementation in order to prevent low order recurrences [19].

The speed of convergence of the iteration depends on the initial guess, for which we use cubic extrapolation in time domain fitting a third degree polynomial through four consecutive values of $\mathbf{C}$. This results usually in an excellent initial guess reducing the sufficient amount of the iterations up to 50%. In the beginning of the ion exchange, we have to use the explicit Euler method [13] to compute the initial guess; the extrapolation is not reliable because of the fast concentration changes within the glass substrate.

3 Adaptive grid and time step

Nonuniform grid spacing in y direction at given time t can be determined by spreading a fixed number of nodes according to a weight function which minimizes the error according to some criteria. In the design of thin diffractive elements for free-space optics, the integral of the concentration over y is the only relevant quantity. It is related to the phase function ϕ by equation

$$\phi(x, z) = \frac{2\pi}{\lambda} \Delta n_{\max} \int_{0}^{p} C(x, y, z) \, \mathrm{d}y, \tag{10}$$

where λ is the vacuum wavelength of light and p is the thickness of the glass substrate.

The estimate for pointwise error can be derived for finite difference algorithms. Applying the Crank-Nicholson method to linear diffusion Eq. (2), the pointwise error estimate per unit time becomes [13]

$$\begin{aligned} &\frac{\partial C}{\partial t} - D\left(\frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2} + \frac{\partial^2 C}{\partial z^2}\right) \\ &\approx \frac{(\Delta t)^2}{12}\frac{\partial^3 C}{\partial t^3} + \frac{D}{12}\left[(\Delta x)^2 \frac{\partial^4 C}{\partial x^4} + (\Delta y)^2 \frac{\partial^4 C}{\partial y^4} + (\Delta z)^2 \frac{\partial^4 C}{\partial z^4}\right], \end{aligned} \tag{11}$$

where Δx, Δy and Δz are node separations in a uniform grid. This estimate holds reasonably well also for the weakly nonlinear case with a non-uniform, slowly changing grid spacing. The error resulting from discretization in y direction can be approximated by estimating the time-average of $\partial^4 C/\partial y^4$ in the nodes. This can be done by using the analytical solution of the one-dimensional linear diffusion Eq. (2) given by

$$C(y) = \operatorname{erfc}\left(\frac{y}{2\sqrt{D_{\mathrm{eff}} t}}\right), \tag{12}$$

where erfc is the complementary error function. Here we have defined an effective diffusion constant as $D_{\mathrm{eff}} = D_A/[0.5(M-1)+1]$ to compensate for the error brought in using linear Eq. (2). This approximation works well as an upper limit to the solution in two or three dimensions, since the concentration C at the surface of the glass is, of course, much lower under the mask than under the apertures.

According to Eq. (11), the cumulative error introduced by discretization in y direction at the point y can be assumed to be proportional to the time-average of the fourth derivative of Eq. (12) with respect to y, denoted by $f(y)$, and the square of the grid spacing Δy. Thus we obtain

$$f(y) = \frac{1}{T}\int_0^T \frac{\partial^4}{\partial y^4}\mathrm{erfc}\left(\frac{y}{2\sqrt{D_{\mathrm{eff}}t}}\right)\mathrm{d}t = \frac{y}{2e^{y^2/(4DT)}\sqrt{\pi T^5 D^5}}, \tag{13}$$

where T is the total ion-exchange time. Now we want to find an optimal node density $g(y)$ such that $\Delta y = 1/g(y)$. The problem is now equivalent to minimizing the functional

$$\int_0^\infty \frac{1}{g^2(y)} f(y)\mathrm{d}y \tag{14}$$

requiring that the number of nodes N is fixed, i.e.,

$$\int_0^\infty g(y)\mathrm{d}y = N. \tag{15}$$

Standard variation calculus yields

$$g(y) = c\sqrt[3]{f(y)}. \tag{16}$$

The constant c can be determined from Eq. (15). The shape of $f(y)$ is always similar to the curve in Fig. 1(a). Because the mask can only slow down the diffusion, we conservatively set the density $g(y)$ to the maximum value between $y = 0$ and $y = y_{\max}$ [Fig. 1(b)]. Sufficient grid depth is automatically determined by Eq. (16), but it can be checked by requiring that the concentration estimated by Eq. (12) at the bottom of the grid does not exceed some maximum value.

To be able to interchange the results of various computations with different grids, we interpolate the final result into a uniform grid. Grid adaptivity in x and z direction would be possible, too, but the case is more complicated in the presence of several mask apertures with variable widths.

Without increasing discretization error in time domain, the time step Δt can be usually increased in the course of computation. Now the third derivative of C with respect to time is approximated by Lagrange interpolation [13] using data from four previous time steps. The first four time steps are computed using small time steps. Then the length of the time step is determined using the maximum value of $\partial^3 C/\partial t^3$ over all nodes. The time step size is then approximated by using Eq. (11) from which we obtain

$$\Delta t = \sqrt{\frac{12E_{\max}}{T[\partial^3 C/\partial t^3]_{\max}}}, \tag{17}$$

where $E_{\max}/T$ is the error tolerance, i.e., the maximum allowed error per unit time. Although the maximum norm may seem to be too careful a choice compared with an average error, it is much safer than using an average norm, e.g., L_1 or L_2.

4 Evaluation of the methods

To compare the efficiency and the accuracy of the implemented numerical methods, the design of a free-space DOE for 1-to-5 beam splitting [7] is considered (Fig. 2). The beam splitter is a periodic diffractive element that divides the incoming laser beam into five equal intensity beams with maximum diffraction efficiency. The grating period $d_x = 123$ μm. The element is fabricated in two steps. Firstly, a glass substrate with one aperture (width 19.7 μm) within the grating period is immersed in a $AgNO_3$ melt for 27300 s. Secondly, the substrate is covered with another mask with one aperture (width 98.4 μm) centered with the previous aperture. The Ag^+–Na^+ ion exchange in the second step is 9000 s. The parameters for the glass are $M = 0.7$, $D_A = 2.0 \cdot 10^{-15}\,\mathrm{m^2/s}$ (at the temperature 343°C), and $\Delta n_{\max} = 0.049$ simulating Ag^+ ion exchange in Corning 0211 glass.

Results (Table 1) are computed using the Rosenbrock method, the explicit non-adaptive Du Fort–Frankel method, and the PR–ADI method. The PR-ADI method is implemented according to Ref. [12] with adaptivity introduced in the time step and the grid spacing in y direction. Because our ion-exchange process is purely thermal, the convection term in Ref. [12] is excluded. The computations with the Rosenbrock method and the PR–ADI are done by using an adaptive grid with 128 points in x direction and 40 points in y direction, but due to symmetry of the solution, only one half of the grid is used in the computation. During the computation only such nodes in y direction are used that are predicted by Eq. (12) to have significant values ($C > 10^{-8}$) for concentration. This greatly reduces the overall computing time. The length of the time step is determined from Eq. (17) by using $E_{\max} = 0.5$, and the initial time step is set to 10 s. Computations with the Du Fort–Frankel method are carried out with a 128×40 and 256×75 nonadaptive grids with constant spacing of the nodes in both directions. In this method, we use constant time steps between 10 s and 120 s. Computations are carried out in the IBM 9076 SP2 computer with a Power2 model 590 processor, which is capable of 270

Mflops.

With 128 nodes in the x direction the spacing of the nodes Δx is 1.0 μm. In the optimization of DOEs, however, better resolution than 1.0 μm in x direction is needed. We have designed the mask supposing that we use laser-beam lithography, and have therefore used spacing of $\Delta x = 0.24$ μm. The last three entries in Table 1 have been computed with this resolution, which corresponds to 512 points in the x direction.

The error criterion of the solution is the root mean square norm

$$\|\phi\| = \sqrt{\int_0^d [\phi(x) - \phi^*(x)]^2 \mathrm{d}x/d}, \tag{18}$$

where ϕ is the computed phase function and ϕ^* is the exact phase function. As an analytic solution cannot be found, the exact phase function is approximated by the result computed with the Rosenbrock method using eight times denser grid and short time steps.

The stability of the Rosenbrock and the PR–ADI methods are found to be very good. The PR–ADI method diverges, if the initial time step is set too long. This, however, does not usually lead to significantly longer computation times compared to the Rosenbrock method, because the time step is rapidly increased during the computation. The Du Fort–Frankel method, for its part, suffers from severe time step restriction due to poor stability, and the computation times are often very long in the case of long ion exchange processes.

The superiority of the implicit methods to the explicit one is clear. In this example, the Rosenbrock method is several decades faster than the explicit Du Fort–Frankel method. The introduced adaptivity in the time step accounts for much of the speedup, since towards the end of the diffusion time steps as large as thousands of seconds can be used. In the Du Fort–Frankel method as large time steps cannot be used because of the poor stability. Therefore, the speedup over the Du Fort–Frankel method can be even greater when processes longer than the one described here are simulated. With the implicit methods better accuracy has also been agained compared to the explicit method. This is because in the Du Fort–Frankel method, the first-order accurate backward difference approximation $C_0 = C_1$ must be used for zero-flux boundary conditions since the stability would be lost using the central difference approximation [20].

5 Application to integrated optics

Although the main motivation for our study was the need for optimization of computer-synthesized DOEs produced by ion exchange, effective process simulation methods could be useful also in integrated optics. When the ion-exchanged waveguide technology is compared to its most important rival, the doped silica glass waveguide technology, the latter has simple waveguide profiles defined by the mask pattern dimensions and the deposited layer thicknesses and refractive indices, while the relationship between ion-exchanged waveguide profiles and fabrication parameters is quite more complicated and obtained only through process simulation [21]. Fast process simulation methods should thus be important in design and optimization of ion-exchanged waveguide devices, too. Although it is possible to design guided-wave devices without extensive optimization, for actual products establishing optimized geometries should be important. Devices can be optimized not only in terms of their optical performance, but also in terms of size, which is important in integrated optics.

In guided-wave devices, the waveguide cross-sections change typically very gradually in the direction of light propagation, which means that ion diffusion in this direction is insignificant. Thus in fabrication process simulation, it is only necessary to solve the two-dimensional ion diffusion problem for the device cross-section. However, with even some complication in device geometry, a very large number of different cross-sections need to be included in the simulation. One typical glass waveguide device is for example 2×2 adiabatic 3-dB coupler [22] shown in Fig. 3. This device has the advantage of polarization and wavelength insensitive operation and is used for example in Mach-Zehnder structures for wavelength division multiplexing [23] and in $2\times$N splitters [24]. Its disadvantage is the rather great length of the coupler. The Fig. 3(a) shows the device geometry, where adiabatic branching occurs by gradual separation of waveguides having different widths. An alternative geometry [25] in Fig. 3(b), analogous in operation, has the two waveguides only brought close to each other in the symmetric part of the junction, and where adiabatic branching occurs by gradually changing the widths of the two waveguides. In order to optimize a coupler, e.g., in terms of device length, geometries need to be studied, where both the widths of the two waveguides and their separation are changing in the adiabatic branch, and neither of these changes need to be linear. For such optimization, cross-sections for given ion exchange process from various mask patterns need to be solved first before optical modeling by, e.g., beam propagation methods [11]. Each mask pattern has two mask openings with different widths having various separations between them, and the number of such different cross-sections to be used in optimization is likely to be thousands.

As an example, we present computation of a typical cross-section for the fabrication process presented in Ref. [23] in Corning 0211 glass [Fig. 3(c)]. The cross-section has 2.5 μm and 5.5 μm wide openings, with 10.0 μm separation between centers of the apertures. Ion exchange time is 750 s, with 1000 s post-bake diffusion. Post-baking means keeping the ion-exchanged glass substrate in a furnace without a salt-melt, i.e., external ion source.

Computation of the non-periodic elements is similar to the periodic diffractive elements, but the boundaries are treated with the zero-flux boundary conditions and the domain is chosen sufficiently large. For the post-bake, zero-flux boundary condition is used at the surface, too. With a 100×60 grid ($\Delta x = 0.5$ μm) and time domain tolerance $E_{\max} = 5 \times 10^{-2}$ we get a local error that is lower than $1.5 \times 10^{-2} C_0$ everywhere in the domain. The overall computing times for the Rosenbrock method are about 0.5 CPUs using either CG, CGS, QMR, or SOR for solving the systems of linear equations. This can be compared with the overall computing time of 5.6 CPUs for the Du Fort–Frankel method using a 200×120 grid ($\Delta x = 0.25$ μm) and a time step of 20 s, which gives a maximum local error of $3.0 \times 10^{-2} C_0$. We note that in this problem, a grid spacing of $x = 0.5$ μm is too coarse for the Du Fort–Frankel method, giving a maximum local error of about $10 \times 10^{-2} C_0$ irrespective of the time step. Since in the optimization hundreds or thousands cross-sections must be computed, the speedup using an implicit finite difference method corresponds to great savings in CPU time.

6 Conclusions

Ion exchange in glass is an important candidate for the fabrication of various micro-optics components. In order to be a competitive technique, optimization methods must be used in the design of ion-exchanged elements. Thus, fast ion-exchange modeling is crucial. In this paper, a fast finite difference method using linearly implicit Rosenbrock method has been implemented for solution of the nonlinear equation. Simulating two- and three-dimensional ion-exchange processes, weak nonlinearity allows linearization of the system of equations without significant detriment in accuracy.

Adaptive time step combined with dynamic error estimation in the course of computation allows increasingly large time steps towards the end of the ion exchange computation. This is especially important in modeling of long ion-exchange processes. The longer the simulation times are, the greater is the decrease in CPU time in comparison with explicit methods. As an example, the simulation of a 10-hour ion-exchange process was accelerated by several decades in comparison to the commonly used explicit Du Fort–Frankel finite difference method. Comparisons were also made with the PR-ADI method, which was found to work well using the adaptivity in the time step and grid spacing. The computation times with PR-ADI are comparable with the Rosenbrock method.

The Rosenbrock method can be implemented for various known forms of the thermal ion exchange equation. With a more complex mathematical model, the computation of the Jacobian becomes more elaborate and is likely to increase overall CPU time. The method can also be extended to include electric-field assisted process. Then QMR or CGS iteration algorithms, which are suitable for nonsymmetric set of equations, are expected to be most useful.

The design of complex ion-exchanged elements is greatly enhanced using the finite difference methods discussed in this paper. We believe that the methods will be useful in design of integrated optics circuits, diffractive free-space elements as well as microlenses. The algorithms were presented in three dimensions, and an interesting point for future research would be modeling of complex waveguide structures by three-dimensional simulation of ion exchange. Our intention is also to design and demonstrate free-space DOEs with two-dimensional diffraction patterns using three-dimensional ion-exchange simulation.

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References

[1] T. Findakly, Opt. Eng. 24 (1985) 244.

[2] R. V. Ramaswamy and R. Srivastava, J. Lightwave Technol. 6 (1988) 984.

[3] S. I. Najafi, ed., Introduction to Glass Integrated Optics (Artech House, Boston, 1992).

[4] M. Oikawa, K. Iga, M. Morinaga, T. Usui, and T. Chiba, Appl. Opt. 23 (1984) 1787.

[5] A. J. Cantor, M. M. Abou el leil, and R. H. Hobbs, Appl. Opt. 30 (1991) 2704.

[6] J. Bähr, K.-H. Brenner, S. Sinzinger, T. Spick, and M. Testorf, Appl. Opt. 33 (1994) 5919.

[7] R.-P. Salmio, J. Saarinen, J. Turunen, and A. Tervonen, Appl. Phys. Lett. 66 (1995) 917.

[8] R.-P. Salmio, J. Saarinen, H. Saarikoski, J. Turunen, and A. Tervonen, in Diffractive Optics and Micro-Optics, Vol. 5, 1996 OSA Technical Digest Series (Optical Society of America, Washington DC, 1996), pp. 39–42.

[9] H. Bach and N. Neuroth, eds., The properties of optical glass, (Springer, Berlin, 1995)

[10] A. Tervonen, in Introduction to Glass Integrated Optics, ed. S. I. Najafi, (Artech House, Boston, 1992), pp. 73–105.

[11] H.-P. Nolting and R. März, J. Lightwave Technol. 13 (1995) 216.

[12] P. J. Masalkar, Optik 95 (1994) 168.

[13] J. H. Ferziger, Numerical Methods for Engineering Application (John Wiley and Sons, New York, 1981).

[14] E. Hairer and G. Wanner, Solving Ordinary Differential Equations II (Springer-Verlag, Berlin, 1991).

[15] G. H Golub and C. F. Van Loan, Matrix Computations (The Johns Hopkins University Press, London, 2nd edition, 1989).

[16] B. A. Carré, Computer J. 4 (1961) 73.

[17] P. Sonneveld, SIAM J. Sci. Stat. Comput. 10 (1989) 36.

[18] R. W. Freund, SIAM J. Sci. Comput. 14 (1993) 470.

[19] H. A. Van der Vorst, SIAM J. Sci. Stat. Comput. 10 (1989) 1174.

[20] L. Lapidus ja G. F. Pinder, Numerical Solution of Partial Differential Equations in Science and Engineering (John Wiley & Sons, Inc., New York, 1982).

[21] A. Tervonen, in SPIE Critical Reviews of Optical Science and Technology CR53, (SPIE - Int. Soc. Opt. Eng., Bellingham, 1994), pp. 25–52.

[22] M. Izutsu, A. Enokihara, and T. Sueta, Opt. Lett. 7 (1982) 549.

[23] A. Tervonen, S. Honkanen, and S. I. Najafi, Opt. Eng. 32 (1993) 2083.

[24] B. Wolf and N. Fabricius, EFOC&N 1994, 12th Annual Conference on European Fibre Optic Communications & Networks, Heidelberg, Germany, June 1994, The European Institute for Communications and Networks, Geneva, pp. 61–64.

[25] R. Adar, C. H. Henry, R. F. Kazarinov, R. C. Kistler, and G. R. Weber, J. Lightwave Technol. 10 (1992) 46.

Fig. 1. (a) Approximation to the distribution of the mean fourth derivate of the concentration with respect to y, i.e., $f(y)$. (b) Approximation Eq. (16) to the density of the grid nodes in y direction that minimizes the error in the phase function Eq. (10).

Fig. 2. Cross-section with equal concentration curves of Ag^{+} ions after (a) the first and (b) the second ion-exchange step for the fabrication of a computer-synthesized diffractive optical element optimized for 1-to-5 beam splitting.

Fig. 3. (a), (b) Schematic top-views of 2×2 adiabatic 3-dB couplers. (c) Cross-section with the equal concentration curves of Ag^{+} ions.

Method	Total CPU time (s)	Error (rad)	Time step (s)	Grid size
Rosenbrock				
CG+ILU	0.50	3.5×10^{-2}	Adaptive	128×40
CGS+ILU	0.62	3.5×10^{-2}	Adaptive	128×40
QMR+ILU	0.57	3.4×10^{-2}	Adaptive	128×40
SOR	0.20	3.5×10^{-2}	Adaptive	128×40
PR–ADI	0.40	3.6×10^{-2}	Adaptive	128×40
Du Fort–Frankel	14.4	5.4×10^{-2}	10	128×40
Du Fort–Frankel	8.5	8.4×10^{-2}	20	128×40
Du Fort–Frankel	9.5	4.2×10^{-2}	80	256×75
Du Fort–Frankel	7.9	5.2×10^{-2}	100	256×75
Du Fort–Frankel	6.8	5.9×10^{-2}	120	256×75
Rosenbrock				
SOR	1.9	2.6×10^{-2}	Adaptive	512×40
Du Fort–Frankel	101.3	3.4×10^{-2}	20	512×150
Du Fort–Frankel	53.0	4.1×10^{-2}	40	512×150

Table 1
Comparison of Rosenbrock method against Du Fort–Frankel and PR-ADI methods for the simulation of the ion-exchanged 1-to-5 beam splitter. Total CPU time and relative error using Eq. (18) are shown for various time steps and grid sizes.