September 10 - 12, 2007
Pilsen, Czech Republic

ON THE THREE FORMULATIONS OF TRANSPARENT BOUNDARIES FOR THE BEAM PROPAGATION METHOD

ĽUBOMÍR ŠUMICHRAST AND MATTHIAS EHRHARDT

Abstract: *For the simulation of the propagation of optical waves in the open waveguiding structures of the integrated optics the beam propagation method of solution of the parabolic wave equation is commonly used. It is of paramount importance to have well-performing transparent boundary conditions applied on the boundaries of the computational window, to enable the superfluous portion of the propagating wave to radiate away from the waveguiding structure. Three different formulations (continuous, semi-discrete and fully-discrete) of the non-local transparent boundary conditions are introduced and compared here.*

Keywords: *Electromagnetic waves, photonic structures, computer simulation, transparent boundary conditions*

INTRODUCTION

For the computer modelling of the propagation of optical waves in the open waveguiding structures of the integrated optics often the scalar parabolic wave equation is used. For a correct solution it is of paramount importance to have appropriate transparent boundary conditions formulated on the boundaries of the computational window, which enable the superfluous portion of the propagating wave to radiate away from the computational window and the waveguiding structure. For the two-dimensional parabolic equation (planar waveguiding structures) usually the continuous transparent boundary condition as formulated by e.g. Baskakov and Popov [1] with its subsequent discretisation has been used for simulations of photonic structures [2]. However, by the *ad hoc* discretisation of the continuous formulae an extra error is introduced. The semi-discrete formulation [3] may improve the situation. Recently published fully-discrete formulation of the transparent boundary conditions [4] is naturally compatible with the fully discrete finite-differences Crank-Nicolson method commonly used in the beam propagation method.

In the case of longitudinally invariant planar structures the propagation of the electromagnetic waves in scalar and parabolic approximation is governed by the Maxwell equations

$$\operatorname{curl}\boldsymbol{E}(\boldsymbol{r},t) = -\mu\frac{\partial \boldsymbol{H}(\boldsymbol{r},t)}{\partial t},\ \operatorname{curl}\boldsymbol{H}(\boldsymbol{r},t) = \varepsilon\frac{\partial \boldsymbol{E}(\boldsymbol{r},t)}{\partial t} \qquad (1)$$

where the electromagnetic field vectors and material constants have their usual meaning. By an usual procedure from (1) the wave equation

$$\nabla^2 f(\boldsymbol{r},t) - \mu\varepsilon\frac{\partial^2 f(\boldsymbol{r},t)}{\partial t^2} = 0 \qquad (2)$$

for any Cartesian component $f(\boldsymbol{r},t)$ of the field vectors $\boldsymbol{E}(\boldsymbol{r},t)$, $\boldsymbol{H}(\boldsymbol{r},t)$ can be obtained. For monochromatic, i.e. harmonically-in-time oscillating wave in the complex representation given by

$$f(\boldsymbol{r},t) = \varphi(\boldsymbol{r})\exp(j\omega t) \qquad (3)$$

one obtains for the complex wave amplitude $\varphi(\boldsymbol{r})$

$$\nabla^2\varphi(\boldsymbol{r}) + \beta^2\varphi(\boldsymbol{r}) = 0\,, \qquad (4)$$

where $\beta = \omega\sqrt{\mu\varepsilon}$ is the propagation constant. If the wave has a particularly developed direction of propagation, say in Cartesian coordinates y, then one can strip-off rapid oscillations in this direction from the complex wave amplitude by the substitution

$$\varphi(x,y,z) = \psi(x,y,z)\exp(-jky)\,. \qquad (5)$$

Then instead of (4) one obtains

$$-2jk\frac{\partial\psi}{\partial y} + \frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} + \frac{\partial^2\psi}{\partial z^2} + \left[\beta^2 - k^2\right]\psi = 0\,. \qquad (6)$$

For wave propagation in homogeneous space, where $\mu,\varepsilon = const$, k can be set equal β and (6) simplifies into

$$-2\mathrm{j}k\frac{\partial\psi}{\partial y}+\frac{\partial^2\psi}{\partial x^2}+\frac{\partial^2\psi}{\partial y^2}+\frac{\partial^2\psi}{\partial z^2}=0\,. \qquad (7)$$

In what follows we shall consider only two-dimensional problems (planar structures), i.e. the spatial coordinate variable z is omitted. If the spatial variations of the wave amplitude are slow compared to the fast oscillations of the carrier frequency, i.e. $\partial\psi/\partial y << k$, then the second derivative with respect to y in (7) can be neglected and one arrives to the wave equation in parabolic approximation (sometimes called the Fresnel equation)

$$-2\mathrm{j}k\frac{\partial\psi}{\partial y}+\frac{\partial^2\psi}{\partial x^2}+\left[\beta^2-k^2\right]\psi=0\,. \qquad (8)$$

The variable x means the transversal coordinate and the wave propagates along the longitudinal coordinate y. In case of waveguiding structures the phase constant β may be a function of the transversal variable, $\beta=\beta(x)$, particularly for homogeneous waveguides it is a kind of by-parts-constant function.

1 CONTINUOUS TRANSPARENT BOUNDARY CONDITIONS

If the equation (8) should be solved numerically the transversal variable x must be bounded to some interval, say $x\in(0,x_{\max})$ called computational window. In course of wave propagation the wave front changes due to the self-diffraction, the wave, in general, diverges (apart of some special cases) and thus also the wavefront originally bounded within the computational window reaches the boundaries and will be out-radiated throughout the computational window. The problem of transparent boundaries consists in formulating such boundary conditions for $\psi(x,y)$ that on the "left" boundary $x=0$ only the wave propagating to the left, and on the "right" boundary $x=x_{\max}$ only the wave propagating to the right exists, i.e. no reflections on the boundaries occur.

The parabolic wave equation (8) can be formally written as

$$\left\{\frac{\partial}{\partial x}-\mathrm{j}\sqrt{\left[\beta^2-k^2\right]-2\mathrm{j}k\frac{\partial}{\partial y}}\right\}\times$$
$$\times\left\{\frac{\partial}{\partial x}+\mathrm{j}\sqrt{\left[\beta^2-k^2\right]-2\mathrm{j}k\frac{\partial}{\partial y}}\right\}\psi=0\,, \qquad (9)$$

and factorised into two one-way wave equations, i.e.

$$\left\{\frac{\partial}{\partial x}-\mathrm{j}\sqrt{\left[\beta^2-k^2\right]-2\mathrm{j}k\frac{\partial}{\partial y}}\right\}\psi=0\,, \qquad (10)$$

$$\left\{\frac{\partial}{\partial x}+\mathrm{j}\sqrt{\left[\beta^2-k^2\right]-2\mathrm{j}k\frac{\partial}{\partial y}}\right\}\psi=0\,, \qquad (11)$$

where each one characterizes the wave propagating either in the $-x$ or in the $+x$ direction with the formal solution

$$\psi(x,y)\approx$$
$$\approx\exp\left\{\pm\mathrm{j}(x-x_0)\sqrt{\left[\beta^2-k^2\right]-2\mathrm{j}k\frac{\partial}{\partial y}}\right\}\psi(x_0,y)\,. \qquad (12)$$

The transparent boundary conditions have to guarantee that the wave amplitude fulfils on the left boundary, $x=0$, relation (12) with the upper sign and on the right boundary, $x=x_{\max}$, the same with the lower sign.

Taking Laplace transform of $\psi(x,y)$ in y-variable, i.e.

$$\Psi(x,p)=\int_0^\infty\psi(x,z)\exp(-py)dy \qquad (13)$$

and substituting into the parabolic wave equation (8) yields

$$-2\mathrm{j}kp\Psi(x,p)+\frac{\partial^2\Psi(x,p)}{\partial x^2}+$$
$$+\left[\beta^2(x)-k^2\right]\Psi(x,p)=0\,. \qquad (14)$$

Solution of (14) reads

$$\Psi_{1,2}(x,p)=$$
$$=\Psi(x_0,p)\exp\left\{\pm\mathrm{j}(x-x_0)\sqrt{\beta^2-k^2-2\mathrm{j}kp}\right\}, \qquad (15)$$

i.e. it consists of two transversally propagating waves, either along the negative (upper sign) or along the positive (lower sign) direction of the x-axis. These two solutions represent in the Laplace transform domain the solution (12) of the two corresponding "one-way" wave equations (11).

Differentiating (15) yields the relation between $\Psi(x,p)$ and its derivative $\partial\Psi(x,p)/\partial x$

$$\frac{\partial\Psi(x,p)}{\partial x}=\mp\Psi(x,p)\sqrt{2\mathrm{j}kp-(\beta^2-k^2)} \qquad (16)$$

or in the form

$$\Psi(x,p)=\mp\frac{1}{\sqrt{2\mathrm{j}kp-(\beta^2-k^2)}}\frac{\partial\Psi(x,p)}{\partial x} \qquad (17)$$

The inverse Laplace transform of (17) yields the convolution integral

$$\psi(x,y)=\frac{\mp1}{\sqrt{2\mathrm{j}\pi k}}\int_0^y\frac{1}{\sqrt{y-\zeta}}\exp\left[-\mathrm{j}\frac{\beta^2-k^2}{2k}(y-\zeta)\right]\times$$
$$\times\frac{\partial\psi(x,\zeta)}{\partial x}d\zeta\,. \qquad (18)$$

If one may set $k=\beta$ then (18) is simplified into

$$\psi(x,y)=\frac{\mp1}{\sqrt{2\mathrm{j}\pi k}}\int_0^y\frac{1}{\sqrt{y-\zeta}}\frac{\partial\psi(x,\zeta)}{\partial x}d\zeta\,. \qquad (19)$$

This formula (19) is called impedance formulation and is identical to the original Baskakov & Popov's formula [1]. In (18) and(19) the values in boundary points $(x,y)=(0,y_0)$, or $(x,y)=(x_{\max},y_0)$ are expressed through the derivative of boundary values in all "previous" boundary points $(x,y)\in(0,0)\div(0,y_0)$, or $(x_{\max},y)\in(x_{\max},0)\div(x_{\max},y_0)$. Thus both formulas (18) and (19) are non-local, which in fact rather complicates their application. On the other hand the initial integration point in (18) and (19) is arbitrary, i.e. the integration path can be, at least conceptually, kept of constant length. Using thus this relation the reflections of waves in the boundary points $x=0$ and $x=x_{\max}$ are prohibited.

2 First discretisation: discrete propagation direction

For the numerical computer simulation the wave amplitude profile $\psi(x,y)$ has to be taken in the set of discrete points (x_m,y_n), $i=0,1,2,\dots,M$, $n=0,1,2,\dots$ yielding thus the set of discrete values. Let us first consider discretisation along the propagation coordinate y, i.e. taking the discrete values of $\psi(x,y)$ in equidistant points $y_n=n\Delta_y$,

$$\psi(x,y_n)=\psi(x,n\Delta_y)=\psi_n(x). \tag{20}$$

Using the implicit Crank-Nicolson strategy the semi-discretised formulation of (8) takes the form

$$-4\mathrm{j}k\frac{\psi_{n+1}(x)-\psi_n(x)}{\Delta_y}+\left[\frac{\partial^2\psi_{n+1}(x)}{\partial x^2}+\frac{\partial^2\psi_n(x)}{\partial x^2}\right]+$$
$$+\left[\beta^2-k^2\right]\left[\psi_{n+1}(x)+\psi_n(x)\right]=0. \tag{21}$$

Instead of Laplace transform (13) for continuous $\psi(x,y)$ it is quite natural to take the Z-transform

$$\Psi(x,z)=\sum_{n=0}^{\infty}\psi_n(x)z^{-n} \tag{22}$$

for the discrete sequence $\{\psi_n(x)\}\big|_{n=0,1,2,..}$. With the "shift" property of the Z-transform (21) yields

$$\frac{\partial^2\Psi(x,z)}{\partial x^2}+\left\{\left[\beta^2-k^2\right]-\frac{4\mathrm{j}k}{\Delta_y}\frac{z-1}{z+1}\right\}\Psi(x,z)=0 \tag{23}$$

with the solution

$$\Psi_{1,2}(x,z)=\Psi(x_0,z)\times$$
$$\times\exp\left\{\pm\mathrm{j}(x-x_0)\sqrt{\beta^2-k^2-\frac{4\mathrm{j}k}{\Delta_y}\frac{z-1}{z+1}}\right\}. \tag{24}$$

In analogy to (16) one obtains

$$\frac{\partial\Psi(x,z)}{\partial x}=\mp\Psi(x,z)\sqrt{\frac{4\mathrm{j}k}{\Delta_y}\frac{z-1}{z+1}-(\beta^2-k^2)} \tag{25}$$

or in the form

$$\Psi(x,z)=\mp\left[\frac{4\mathrm{j}k}{\Delta_y}\frac{z-1}{z+1}-(\beta^2-k^2)\right]^{-1/2}\frac{\partial\Psi(x,z)}{\partial x}, \tag{26}$$

or in case $k=\beta$

$$\Psi(x,z)=\mp\left[\frac{4\mathrm{j}k}{\Delta_y}\frac{z-1}{z+1}\right]^{-1/2}\frac{\partial\Psi(x,z)}{\partial x}. \tag{27}$$

Since the values f_n in the Z-transform

$$F(z)=\sum_{n=0}^{\infty}f_nz^{-n} \tag{28}$$

are in fact the coefficients of the Taylor series in variable $1/z$ of $F(z)$ and to the product $G(z)=F(z)H(z)$ in the Z-domain corresponds the discrete convolution of originals

$$g_n=\sum_{k=0}^{n}f_{n-k}h_k, \tag{29}$$

one needs to obtain the Taylor series coefficients in case (26) of the term

$$H(z)=\left[\frac{4\mathrm{j}k}{\Delta_y}\frac{z-1}{z+1}-(\beta^2-k^2)\right]^{-1/2} \tag{30}$$

or in the case (27) of the term

$$H(z)=\sqrt{(z+1)/(z-1)}. \tag{31}$$

As shown in [3]

$$\sqrt{(z+1)/(z-1)}=\sum_{n=0}^{\infty}h_nz^{-n} \tag{32}$$

holds with

$$\{h_n\}=\left\{1,1,\frac{1}{2},\frac{1}{2},\frac{1\cdot3}{2\cdot4},\frac{1\cdot3}{2\cdot4},\frac{1\cdot3\cdot5}{2\cdot4\cdot6},\frac{1\cdot3\cdot5}{2\cdot4\cdot6},\dots\right\}. \tag{33}$$

The resulting discrete convolution formula then reads

$$\psi_n(x)=\sum_{k=0}^{n}\frac{\partial\psi_{n-k}(x)}{\partial x}h_k. \tag{34}$$

3 Second discretisation: discrete transversal direction

The second discretisation yields a two-dimensional array of values

$$\psi(x_m,y_n)=\psi(m\Delta_x,n\Delta_y)=\psi_m^n \tag{35}$$

for $m\in(0,M)$, where Δ_x and Δ_y are (in our case equidistant) discretisation intervals. The computational window is $(0,x_{\max})=(0,M\Delta_y)$. Using the central second differences in Crank-Nicolson discretisation scheme one arrives to the discrete formula analogous to (21)

$$-4\mathrm{j}k\frac{\psi_m^{n+1}-\psi_m^n}{\Delta_y}+$$

$$+\left[\frac{\psi_{m+1}^{n+1}-2\psi_m^{n+1}+\psi_{m-1}^{n+1}}{\Delta_x^2}+\frac{\psi_{m+1}^{n}-2\psi_m^{n}+\psi_{m-1}^{n}}{\Delta_x^2}\right]+$$

$$+\left[\beta^2-k^2\right]\left[\psi_m^{n+1}+\psi_m^n\right]=0\,. \quad (36)$$

This Crank-Nicholson formula is known to conserve power within the computational window and therefore it is especially suitable for the wave propagation computations.

After again having (36) Z-transformed in the propagation direction one obtains the discrete pendant to (23)

$$\frac{\Psi_{m+1}(z)-2\Psi_m(z)+\Psi_{m-1}(z)}{\Delta_x^2}+$$

$$+\left\{\left[\beta^2-k^2\right]-\frac{4\mathrm{j}k}{\Delta_y}\frac{z-1}{z+1}\right\}\Psi_m(z)=0\,. \quad (37)$$

The solution to this difference equation of the second order is

$$\Psi_m(z)=\left\{1-A(z)\pm\sqrt{[1-A(z)]^2-1}\right\}\Psi_{m-1}(z)\,, \quad (38)$$

where

$$A(z)=\Delta_x^2\left\{\frac{\beta^2-k^2}{2}-\frac{2\mathrm{j}k}{\Delta_y}\frac{z-1}{z+1}\right\}. \quad (39)$$

For the simple case $k=\beta$ one obtains

$$A(z)=-\frac{2\mathrm{j}k\Delta_x^2}{\Delta_y}\frac{z-1}{z+1}\,. \quad (40)$$

The analytical inversion of (39), (40) has been obtained in [4] where also thorough analysis of various rather subtle mathematical aspects of the technique is presented.

The resulting formula in form of a convolution is now

$$\psi_m^n=\sum_{k=0}^{n}\psi_{m-1}^{n-k}h_k\,, \quad (41)$$

where

$$1-A(z)\pm\sqrt{[1-A(z)]^2-1}=\sum_{n=0}^{\infty}h_n z^{-n}\,. \quad (42)$$

4 NUMERICAL IMPLEMENTATION

For numerical simulations solely the full Crank-Nicolson formula (36) is used. It can be written in the form

$$D\psi_2^{n+1}-E\psi_1^{n+1}=A\psi_2^n-B\psi_1^n+C\psi_0^n-F\psi_0^{n+1}\,, \quad (43)$$

$$D\psi_{m+1}^{n+1}-E\psi_m^{n+1}+F\psi_{m-1}^{n+1}=$$
$$=A\psi_{m+1}^n-B\psi_m^n+C\psi_{m-1}^n\,,\quad m=2,3,\dots,M-2\,, \quad (44)$$

$$-E\psi_{M-1}^{n+1}+F\psi_{M-2}^{n+1}=$$
$$=A\psi_M^n-B\psi_{M-1}^n+C\psi_{M-2}^n-D\psi_M^{n+1}\,, \quad (45)$$

i.e. the unknowns ψ_i^{n+1}, $i=1,2,\dots,M-1$ on the left sides of (43)-(45) are expressed by the known values in the previous layer ψ_i^n, $i=0,1,2,\dots,M$ and by the must-be-known boundary values ψ_0^{n+1}, ψ_M^{n+1}. This is an implicit type of discretisation scheme, i.e. it requires the solution of a tridiagonal system of equations for each step in the propagation direction y.

All three formulas (18), (34) and (41) can be easily embodied into the Crank-Nicholson scheme. The values of continuous x-derivatives in (18) and in (41) must be in boundary points first approximated by their discrete two-point, or three-point counterparts.

$$\delta\psi_0^n=\partial\psi(x,y_n)/\partial x\big|_{x=0}\approx(\psi_1^n-\psi_0^n)/\Delta_x \quad (46)$$

$$\delta\psi_0^n=\partial\psi(x,y_n)/\partial x\big|_{x=0}\approx$$
$$\approx(-\psi_2^n+4\psi_1^n-3\psi_0^n)/2\Delta_x \quad (47)$$

$$\delta\psi_M^n=\partial\psi(x,y_n)/\partial x\big|_{x=x_{\max}}\approx(\psi_M^n-\psi_{M-1}^n)/\Delta_x \quad (48)$$

$$\delta\psi_M^n=\partial\psi(x,y_n)/\partial x\big|_{x=x_{\max}}\approx$$
$$\approx(3\psi_M^n-4\psi_{M-1}^n+\psi_{M-2}^n)/2\Delta_x \quad (49)$$

If using (18) the approximate values of derivatives in the boundary points are linearly interpolated along the y-direction, i.e. for $y\in(y_{n-1},y_n)$

$$\left.\frac{\partial\psi(x,y)}{\partial x}\right|_{x=0}\approx$$
$$\approx\frac{\delta\psi_0^n(y-y_{n-1})+\delta\psi_0^{n-1}(y_n-y)}{y_n-y_{n-1}}=\Phi_0^n(y) \quad (50)$$

and substituted into (18) with the result for the N-th computational layer

$$\psi_0^N=\frac{\mp 1}{\sqrt{2\mathrm{j}\pi k}}\sum_{n=1}^{n=N}\int_{y_{n-1}}^{y_n}\frac{1}{\sqrt{y_N-\zeta}}\times$$
$$\times\exp\left[-\mathrm{j}\frac{\beta_0^2-k^2}{2k}(y_N-\zeta)\right]\Phi_0^n(\zeta)d\zeta \quad (51)$$

After the integration one obtains ψ_0^N related to ψ_1^N and to all pairs of previous values ψ_0^n and ψ_1^n, $n=0,1,2,\dots N-1$. The unknown value of ψ_0^N expressed by the known values ψ_0^n and ψ_1^n, $n=0,1,2,\dots N-1$ and unknown value ψ_1^N can be then inserted into (43) and ψ_1^N shifted again to the left side to unknowns. For example for the first step the integration domain in (51) spans over of only one step in the y-direction with the result

$$\psi_0^1=\frac{D}{3+4D}\left[4\psi_1^1+2\left(\psi_1^0-\psi_0^0\right)\right] \quad (52)$$

where $D = \sqrt{\Delta_y / 2\pi j k \Delta_x^2}$. Analogous formulas can be obtained for the "right" boundary point $x = x_{\max}$.

As already mentioned the main drawback of all three formulations is the non-locality of the boundary conditions, i.e. for the successful application of the TBC one has to keep track of all previous derivatives in boundary points $\delta\psi_0^n$, $\delta\psi_M^n$, $n = 0,1,2,\ldots N-1$ up to the actually calculated layer $n = N$.

5 RESULTS OF NUMERICAL COMPUTATION

We illustrate the performance of the continuous and semi-discrete boundary conditions using the case of an asymmetrical photonic slab waveguide with the waveguiding slab thickness of 1.0 μm with the refractive index $n_g = 3.24$ (the characteristic value

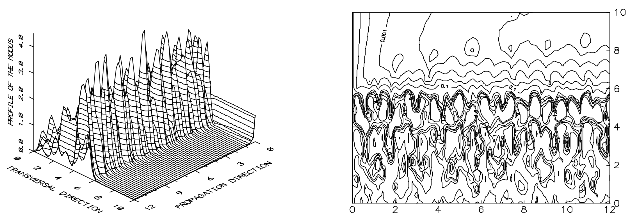

Fig. 1 - *Illustrative results to Table I first column*

for GaAs-InP semiconductor waveguides) with the refractive index of the substrate $n_1 = 3.16$ and the refractive index of the superstrate equal to $n_2 = 2.0$. The fundamental mode of this waveguide is given by

$$\psi(x,y) = \exp(-j\eta y)\begin{cases} \cos(qa-\zeta)\exp(\kappa_1 x), & x < -a \\ \cos(qx+\zeta), & |x| < a \\ \cos(qa+\zeta)\exp(-\kappa_2 x), & x > a \end{cases} \quad (53)$$

In our case $a = 0.5$ μm and for the commonly used free-space wavelength of used radiation $\lambda_0 = 1.5$ μm one obtains the exact values of the $q = 2.14325$ μm^{-1}, $\kappa_1 = 2.09522$ μm^{-1}, $\kappa_2 = 10.4601$ μm^{-1}, $\zeta = 0.29725$ rad with

$$\eta = \beta_g^2 - q^2 - k^2 / 2k \quad (54)$$

depending on the arbitrarily chosen value of *k*, where $\beta_g = 2\pi n_g / \lambda_0$. The modus profile is the exact solution of the full wave equation

$$\frac{\partial^2\psi(x,y)}{\partial x^2} + \frac{\partial^2\psi(x,y)}{\partial y^2} + \beta^2(x)\psi(x,z) = 0 \quad (55)$$

with $\eta = \sqrt{\beta_g^2 - q^2} - k^2$. For the above parameters $\sqrt{\beta_g^2 - q^2} = 0.16588$ μm^{-1}. The width of the computational window was taken $b = 1.0$ μm with Gaussian input profile distribution in the form

$$\psi(x,0) = \exp\left(-x^2 / W_0^2\right) \quad (56)$$

where W_0 is the effective width of the Gaussian profile.

For benchmark simulations it was taken either much larger than the modus profile with $W_0 = 5$ μm, or much smaller with $W_0 = 0.05$ μm, representing thus either nearly a plane wave with nearly constant distribution within the computational window or the excitation by nearly point source of the spherical wave.

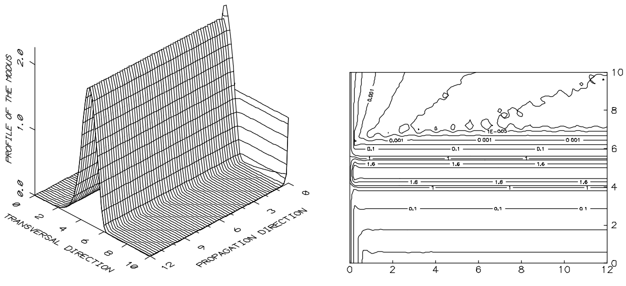

Fig. 2 - *Illustrative results for Table I second column*

The accuracy of calculation was assessed by calculating the correlation factor between exact modus profile and simulated propagating wave profile. The illustrative results of computations are presented in Figures 1 through 3 and the differences of the correlation from the unity are presented in Tables I through IV. In Table I and II the waveguide was excited by the broad Gaussian profile wave (nearly the plane wave) while in the Table III and IV by the narrow Gaussian profile wave (nearly the spherical wave).

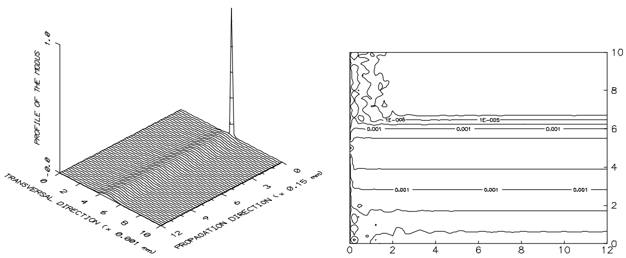

Fig. 3 - *Illustrative results for Table III first column*

Table I

Correlation difference from unity for nearly plane wave

Propagation length 1.8 mm with 2400 steps			
	formula (18)	formula (33)	formula (19)
k = 13.23	.7769D-05	.5247D-4	.5395D-03
k = 8.37	.7384D-01	.8852D-2	.1972D-02
k = 13.57	.2505D-04	.9821D-3	.4496D-03
k = 13.40	.2337D-04	.7772D-3	.4941D-03

The numerical results presented in Table I are for $\Delta_y = \lambda/2$ for the propagation length $y = 1800$ μm, i.e. total of 2400 steps had been calculated. In Table II $\Delta_y = \lambda/16$ for the propagation length $y = 1800$ μm, i.e. total of 19200 steps had been calculated. In the Table III and IV again $\Delta_y = \lambda/2$ and $\Delta_y = \lambda/16$ for $y = 5400$ μm, i.e. for 7200 and 57600 steps respectively. The results indicate that the performance of the transparent boundary conditions depends in all cases strongly on the choice of the constant *k*.

Table II

Correlation difference from unity for nearly plane wave

Propagation length 1.8 mm with 19200 steps			
	formula (18)	formula (33)	formula (19)
k = 13.23	.6363D-05	.3588D-04	.5485D-03
k = 8.37	.2471D+00	.9652D-03	.1354D-04
k = 13.57	.2303D-04	.9952D-04	.1979D-03
k = 13.40	.3190D-03	.4468D-04	.2140D-04

Table III

Correlation difference from unity for nearly spherical wave

Propagation length 5.4 mm with 7200 steps			
	formula (18)	formula (33)	formula (19)
k = 13.237	.9673D-03	.1855D-03	.2386D-03
k = 8.377	.1295D-02	.1777D-03	.1933D-02
k = 13.578	.9716D-03	.2777D-03	.2847D-03
k = 13.405	.1042D-02	.1255D-03	.2406D-03

Table IV

Correlation difference from unity for nearly spherical wave

Propagation length 5.4 mm with 57600 steps			
	formula (18)	formula (33)	formula (19)
k = 13.23	.5627D-04	.4842D-04	.4969D-04
k = 8.377	.1338D-04	.5247D-01	.3259D+00
k = 13.57	.4903D-04	.5528D-4	.6465D-04
k = 13.40	.5092D-04	.5996D-04	.6435D-04

6 CONCLUSIONS

Preliminary numerical results for the asymmetric slab waveguide using the formulae (34) for semi-discrete formulation of transparent boundary condition (TBC) in connection with (31) and (33) as well as the results using the discretised continuous TBC accordingly (18) and (19) show that the performance of the transparent boundary conditions is in a complicated way dependent on many factors as e.g. the step length Δ_y, total number of steps, nature of excitation etc. There is no substantial difference between the performances of respective TBC even if the nonzero term $\beta^2 - k^2$ is not taken into account. No simple recipe can be given as for the prediction of the performance. In all cases the worst performance shows the case when $k = 8.37758$. However for the sufficiently small Δ_y the correlation between the stationary distribution after sufficiently long propagation path and exact modus profile is satisfactory for methods used. Anyhow the formula with $\beta^2 - k^2$ term performed better always when the value of the constant *k* has been chosen in such a way that the oscillations of the slowly varying envelope were significant. In this series of simulations the semi-discrete method with embodied $\beta^2 - k^2$ term was not used yet, neither was used the third (fully discrete formulation) method. Their properties require further investigation. A thorough review and some outlook of mathematical aspects of TBC can be found in recent publication [5].

7 ACKNOWLEDGEMENT

The first author has been supported by the grant No. 1/4085/07 of the Slovak grant agency VEGA. DFG Research Centre MATHEON has supported the second author. Financial support is kindly acknowledged.

8 REFERENCES

[1] V. A. Baskakov, A. V. Popov: "Implementation of Transparent Boundaries for Numerical Solution of the Schrödinger Equation", *Wave Motion*, Vol.14, 1991, pp. 123-128.

[2] R. Accornero, M. Artiglia, G. Coppa, P. DiVitta, G. Lapenta, M. Potanza, P. Ravetto: "Finite Difference Methods for the Analysis of Integrated Optical Waveguides", *Electronics Lett.*, Vol. 26, 1990, pp. 1959-1960.

[3] D. Yevick, T. Friese, F. Schmidt: " A Comparison of Transparent Boundary Conditions for the Fresnel Equation", *J. Comp. Phys.*, Vol. 168, 2001, pp. 433-444

[4] M. Ehrhardt: "Discrete artificial Boundary Conditions", *PhD dissertation*, TU Berlin, 2001.

[5] X. Antoine, A. Arnold, Ch. Besse,M. Ehrhardt, A. Schädle: "A Review of Transparentand Artificial Boundary Conditions Techniques for Linear and Nonlinear Schrödinger Equations", Preprint No. 18, 2007, Institute of Mathematics, TU Berlin, submitted to *Appl. Num. Math.*

Doc. Ing. Ľubomír Šumichrast CSc, Institute of Electromagnetic Theory, Slovak University of Technology, Ilkovičova 3, SK-81219 Bratislava. Slovakia, E-mail: lubomir.sumichrast@stuba.sk

Doz. Dr. Matthias Ehrhardt, Institut für Mathematik, Technische Universität Berlin, Strasse des 17. Juni 136, D-10623 Berlin, Germany, E-mail: ehrhardt@math.tu-berlin.de