UDC 517.9:532.5:519.61
Original scientific paper
Received: 12.12.2012.

Nonlinear macromodel based on Krylov subspace for micromixer of the microfluidic chip

Xueye Chen(1)**, Hong Zeng**(1)**, Hongxiang Wang**(1) and **Jingliang Li**(2)

(1)Faculty of Mechanical Engineering and Automation, Liaoning University of Technology, Jinzhou 121001, CHINA
e-mail: xueye_chen@126.com
(2)The Key Laboratory for Micro/Nano Technology and System of Liaoning Province,
Dalian University of Technology, Dalian 116024, CHINA

SUMMARY

The simulation of MEMS (Micro-Electro-Mechanical-System) containing fluid field could not be well performed by conventional numerical analysis methods. The micro flow field characteristics can be simulated by using macromodel including a nonlinear analysis. This paper set up the macromodel of the micromixer of the microfluidic chip using Krylov subspace projection method. The system functions were assembled through finite element analysis using COMSOL. We took the flow field-concentration field analysis for micromixer finite element model. The finite element functions order is reduced by second-order Krylov subspace projection method based on Lanczos algorithm. It can be shown that the simulation results obtained by using the macromodel are highly consistent with the results of finite element analysis. The calculation using the macromodel is two orders of magnitude faster than the calculation performed by the finite element analysis method. This macromodel should facilitate the design of microfluidic devices with sophisticated channel networks.

Key words: *macromodel, Krylov subspace, micromixer, MEMS.*

1. INTRODUCTION

Considerable effort has been put to the development of microfluidic systems for performing biological and biochemical mixing [1, 2]. Micromixers, an important branch of MEMS (Micro-Electro-Mechanical-System), have as complex a structure and physics field as other MEMS. The development of technologies in the field of Microsystems has generated a wideswpread interest in exploring fast and accurate design methods to simulate entire systems. The typical MEMS can complete many tasks under certain conditions. Multi-physics fields in MEMS make it difficult to design structure especially if these contain a flow field. In MEMS, the coupled effect commonly takes place among mechanical, electrical, fluidic, magnetic and thermal fields [3-6]. The strongly nonlinear effect is usually intractable [7]. In order to design MEMS, finite element and finite volume methods have been successfully applied. These numerical methods are highly effective and accurate but laborious and time consuming, i.e. a solution of three-dimensions Joule heating dispersion by using the finite element method can cost four days and four GB of physical memory [8]. Such computational cost is prohibitive for system-level design of complex microfluidic chips system. Furthermore, when the designed system contains conversion of different signals, such as of non-electric signals to electric signals or other signal processing units, the finite element or finite volume methods are powerless. In order to solve these mentioned problems, the macromodel technologies have been widely investigated in the past few years [9, 10].

The macromodel, also called the reduced order model, is a low-order behavioural representation of a device. The macromodel can be described with hardware language and directly applied to EDA (Electronic Design Automation) environment. Analytical solution [11] and numerical solution [12] are two methods for creating the macromodel. The matrix subspace projection based on matrix transformation is a common numerical method for extracting macromodel from the finite element analysis.

In this work, Lanczos algorithm is applied in setting up the second-order Krylov subspace. We have directly projected a large-scale sparse matrix to the subspace. The algorithm has been tested on the model of the micromixer of the microfluidic chip. The results obtained by the macromodel, when compared with the results obtained by applying the finite element method to the micromixer of the microfluidic chip, shows that the model is completly accurate.

2. THEORETICALY BACKGROUND

The static and dynamic behaviours of MEMS is presented by partial differential equations (PDEs) and corresponding boundary conditions. Discretization using finite element method, finite volume method or finite difference method can transfer PDEs to ordinary differential equations (ODEs), which can be written in the following state-space form:

$$\boldsymbol{\Omega}:\begin{cases}\dot{\boldsymbol{x}}(t)=\boldsymbol{A}\cdot\boldsymbol{x}(t)+\boldsymbol{B}\cdot\boldsymbol{u}(t)\\ \boldsymbol{y}(t)=\boldsymbol{C}\cdot\boldsymbol{x}(t)\end{cases}\tag{1}$$

where, $\boldsymbol{A}\in R^{m\times m}$ is the system matrix, $\boldsymbol{B}\in R^{m\times n}$ is input matrix, $\boldsymbol{C}\in R^{q\times m}$ is output matrix, $\boldsymbol{u}\in R^{n}$ is input variable. $\boldsymbol{y}\in R^{q}$ is output variable and $\boldsymbol{x}\in R^{m}$ is state variable. We replace $\boldsymbol{x}=V\cdot z$, $V\in R^{m\times r}$, $z\in R^{r}$. The dimensionless column vectors of transition matrix $\boldsymbol{V}$, whose number is r, can compose a basis subspace, called projection subspace. If $r<<m$, then the r-dimensional vector z can be considered as the reduced order state variable. The reduced order state function is:

$$\begin{cases}\dot{z}(t)=\hat{\boldsymbol{A}}\cdot z(t)+\hat{\boldsymbol{B}}\cdot\boldsymbol{u}(t)\\ \hat{\boldsymbol{y}}(t)=\hat{\boldsymbol{C}}\cdot z(t)\end{cases}\tag{2}$$

where, $\hat{\boldsymbol{A}}=\boldsymbol{V}^{-1}\boldsymbol{A}\boldsymbol{V}$, $\hat{\boldsymbol{B}}=\boldsymbol{V}^{-1}\boldsymbol{B}$, $\hat{\boldsymbol{C}}=\boldsymbol{C}\boldsymbol{V}$. Performing a Laplace transform for Eq. (1), we can obtain its frequency domain transfer function $\boldsymbol{H}(s)$ by:

$$\boldsymbol{H}(s)=\boldsymbol{C}\cdot(s\boldsymbol{I}-\boldsymbol{A})^{-1}\cdot\boldsymbol{B}=-\boldsymbol{C}\cdot\boldsymbol{A}^{-1}(I-sA^{-1})\boldsymbol{B}\tag{3}$$

Finding a suitable transition matrix $\boldsymbol{V}$ is the key of matrix subspace projection method for the reduction of the original system order. In order to apply Eq. (2) to reduce the order of Eq. (1), $min\|\boldsymbol{y}-\hat{\boldsymbol{y}}\|$ and $min\|\boldsymbol{H}(s)-\hat{\boldsymbol{H}}(s)\|$ in time and frequency domain, respectively, must be satisfied.

An r-dimension Krylov subspace $\boldsymbol{\varphi}_r$ is defined as follows:

$$\boldsymbol{\varphi}_r(\boldsymbol{A}_1,\boldsymbol{b}_1)=span\left\{\boldsymbol{b}_1,\boldsymbol{A}_1\boldsymbol{b}_1,\cdots\boldsymbol{A}_1^{r-1}\boldsymbol{b}_1\right\}\tag{4}$$

where, $\boldsymbol{A}_1\in R^{m\times m}$, $\boldsymbol{b}_1\in R^{m}$ is called starting vector.

Lanczos algorithm [13] can convert large linear equations to tri-diagonal equations and create the orthonormal vectors, makig it possible to construct the unit basic Krylov subspace. The Lanczos process is represented with the chart given in Figure 1.

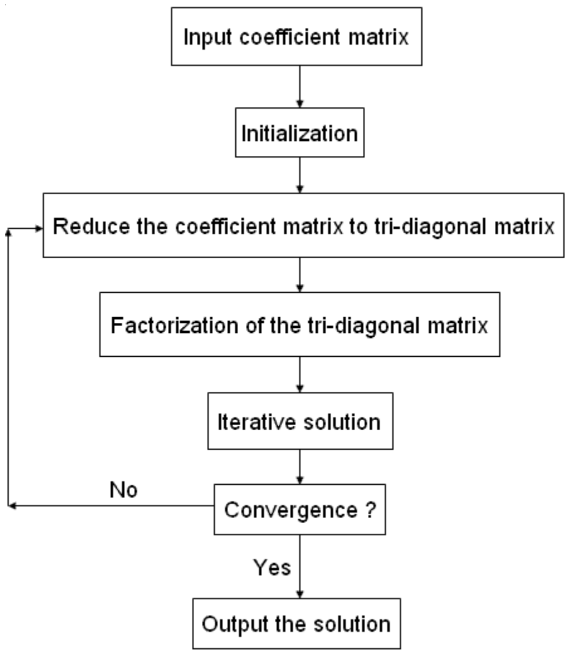

Fig. 1 The flow chart of Lanczos algorithm

The tri-diagonal process is in fact a similarity transformation, and can be expressed by:

$$\boldsymbol{V}_n^{-1}\boldsymbol{A}\boldsymbol{V}_n=\boldsymbol{T}_n\tag{5}$$

We can simplify Eq. (3) to:

$$\begin{aligned}\boldsymbol{H}(s)&=-\boldsymbol{C}\cdot\boldsymbol{A}^{-1}(I-sA^{-1})\boldsymbol{B}=\\&=\boldsymbol{C}\cdot(-\boldsymbol{A}^{-1})\cdot(\boldsymbol{I}-s\boldsymbol{V}_n\boldsymbol{T}_n\boldsymbol{V}_n^{-1})\boldsymbol{B}=\\&=\boldsymbol{C}\cdot\boldsymbol{A}^{T}\cdot\boldsymbol{B}i_1^{T}\cdot(\boldsymbol{I}-s\boldsymbol{T}_n)^{-1}\cdot i_1\end{aligned}\tag{6}$$

where $i\in R^{n}$ is the first standard orthogonal basis in orthogonal basis set $w_i^T\cdot v_j=0,\ i\neq j$. So, we can obtain the moment of the transition function of initial system, $m_i=-\boldsymbol{A}^{-1}\boldsymbol{B}i_1^{T}\cdot\boldsymbol{T}_n^{i}\cdot i_1$. The transition function of the reduced system becomes:

$$\boldsymbol{H}_r(s)=\boldsymbol{A}^{-T}\boldsymbol{B}i_1^{T}(\boldsymbol{I}-s\boldsymbol{T}_r)^{-1}\cdot i_1\tag{7}$$

where $\boldsymbol{T}_r$, is the first $r\times r$ sub-matrix of $\boldsymbol{T}_n$, and $i_1\in R^{r}$ is the first standard orthogonal basis.

If the transition matrix $\boldsymbol{V}$, obtained from Lanczos process is a unit basic Kyle subspace [14], and the first r moments between $\boldsymbol{H}(s)$ and $\hat{\boldsymbol{H}}(s)$ are matching then we can obtain the minimum of $\|\boldsymbol{H}(s)-\hat{\boldsymbol{H}}(s)\|$. Therefore, the original system function matrix can be projected to Krylov subspace and the order can be reduced.

In many engineering problems, second order differential functions are used for describing the dynamical behaviour of a system, as below:

$$\begin{cases} \boldsymbol{M}\ddot{\boldsymbol{x}}(t)+\boldsymbol{E}\dot{\boldsymbol{x}}(t)+\boldsymbol{K}\boldsymbol{x}(t)=\boldsymbol{B}\boldsymbol{u}(t) \\ \boldsymbol{y}(t)=\boldsymbol{C}^T\boldsymbol{x}(t) \end{cases} \tag{8}$$

where, $\boldsymbol{M}$, $\boldsymbol{E}$, $\boldsymbol{K}\in R^{m\times m}$, $\boldsymbol{B}\in R^{m\times n}$, $\boldsymbol{C}\in R^{q\times m}$, $\boldsymbol{u}\in R^n$, $\boldsymbol{y}\in R^q$ and $\boldsymbol{x}\in R^m$. The second order Krylov subspace can be defined by:

$$\boldsymbol{\varphi}_r(\boldsymbol{A}_1,\boldsymbol{A}_2,\boldsymbol{b}_1)=span\{\boldsymbol{k}_0,\boldsymbol{k}_1,\cdots\boldsymbol{k}_{r-1}\} \tag{9}$$

where, $\boldsymbol{k}_0=\boldsymbol{b}_1$, $\boldsymbol{k}_1=\boldsymbol{A}_1\boldsymbol{b}_1$, $\boldsymbol{k}_i=\boldsymbol{A}_1\boldsymbol{k}_{i-1}+\boldsymbol{A}_2\boldsymbol{k}_{i-2}$, and $\boldsymbol{A}_1\boldsymbol{A}_2\in R^{m\times m}$, $\boldsymbol{b}_1\in R^m$. $\boldsymbol{b}_1$ is called the starting vector and $\boldsymbol{k}_i$ is called the basic vector. The preconditioned Lanczos process [15] can be used for creating the second order Krylov subspace, which is, in turn, used to project the dynamic behaviour of a system. As for the projection $\boldsymbol{x}=\boldsymbol{G}\boldsymbol{x}_r$, $\boldsymbol{G}\in R^{m\times r}$, $r<<m$, if one $\boldsymbol{P}\in R^{m\times r}=\boldsymbol{G}$, the first r moments of the original second order system and the reduced order model can match and we obtain the following reduced system:

$$\begin{cases} \boldsymbol{P}^T\boldsymbol{M}\boldsymbol{G}\ddot{\boldsymbol{x}}_r(t)+\boldsymbol{P}^T\boldsymbol{E}\boldsymbol{G}\dot{\boldsymbol{x}}_r(t)\boldsymbol{P}^T\boldsymbol{K}\boldsymbol{G}\boldsymbol{x}_r(t)=\boldsymbol{P}^T\boldsymbol{B}\boldsymbol{u}(t) \\ \boldsymbol{y}=\boldsymbol{C}^T\boldsymbol{G}\boldsymbol{x}_r \end{cases} \tag{10}$$

3. MICROMIXER FINITE ELEMENT MODEL

Micromixer is one of the important components in Micro Total Analysis System and Lab on a Chip. Rapid mixing is essential in many of the microfluidic systems used in biochemical analysis, drug delivery and sequencing or synthesis of nucleic acids. The investigation of micromixers is fundamental to understanding transport phenomena on the microscale. The micromixer fabricated in our laboratory is shown in Figure 2. The outside measurements of the chip are *50 mm* (lenght) $\times$ *25 mm* (width). The width of the micro-channel is *300 microns* and the depth is *30 microns*. The micro-channel was fabricated from a PMMA (polymethyl methacrylate) substrate by hot embossing, and sealed with an other PMMA cover plate enclosing the microchannel. The micromixer can perform mixing by utilizing the “split and recombine” principle. Since the thickness of the microchanel is much smaller than length and width, we consider it as a plane problem and mesh it with 2D element.

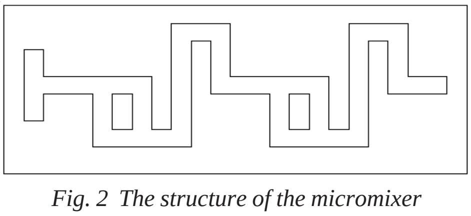

Fig. 2 The structure of the micromixer

The finite element micromixer model is coupled with mechanical, fluidic and concentration fields, therefore, it is a strongly nonlinear problem. The finite element analysis contains three steps. Firstly, the incompressible Navier-Stokes equation, Eq. (11), and continuity equation, Eq. (12), are solved in order to get the velocity field:

$$\frac{\partial \boldsymbol{v}}{\partial t}+\boldsymbol{v}\cdot\nabla\boldsymbol{v}=f-\frac{1}{\rho}\nabla\boldsymbol{P}+\mu\Delta\boldsymbol{v} \tag{11}$$

$$\nabla\cdot\boldsymbol{v}=0 \tag{12}$$

where, $\boldsymbol{v}$ is the velocity vector, f is the body force, ρ is the density of the fluid, $\boldsymbol{P}$ is the pressure and μ is the dynamic viscosity of the fluid. Secondly, the concentration distribution can be calculated from convection–diffusion equation, Eq. (13), after obtaining the velocity field:

$$\frac{\partial\phi}{\partial t}+(\boldsymbol{v}\cdot\nabla)\phi=D\nabla^2\phi \tag{13}$$

where, ϕ is the concentration of species, D is the diffusion coefficient and v is the fluid velocity. Then, the concentration can be used for investigating the degree of fluid mixing by equation:

$$\gamma(x)=1-\frac{\int_0^W|\phi-\phi_\infty|dy}{\int_0^W|\phi_0-\phi_\infty|dy}\times 100\% \tag{14}$$

where, W is the width of the micro-channel, ϕ is the concentration of species across the width of the mixing channel, ϕ_0 and ϕ_∞ are the sample concentration profiles with completely unmixed (*0* or *1*) and completely mixed states (*0.5*), respectively.

The finite element model of the micromixer is set up using COMSOL software. The mesh model is shown in Figure 3. The number of elements and nodes are *3936* and *5095* respectively.

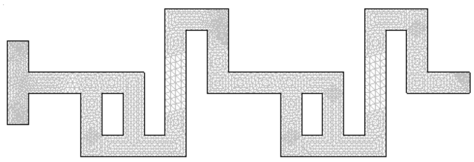

Fig. 3 The finite element model of the micromixer

We have solved the coupling problem by using COMSOL's sequential coupling. The coupling in the matrix equation is shown as:

$$\begin{bmatrix} \boldsymbol{M} & 0 \\ 0 & 0 \end{bmatrix}\begin{bmatrix} \ddot{\boldsymbol{u}} \\ \ddot{\boldsymbol{\varphi}} \end{bmatrix}+\begin{bmatrix} \boldsymbol{D} & \boldsymbol{0} \\ \boldsymbol{D}^{U\phi} & \boldsymbol{D}^{\phi} \end{bmatrix}\begin{bmatrix} \dot{\boldsymbol{u}} \\ \dot{\boldsymbol{\varphi}} \end{bmatrix}+\begin{bmatrix} \boldsymbol{K} & \boldsymbol{K}^{U\phi} \\ 0 & \boldsymbol{K}^{\phi} \end{bmatrix}\begin{bmatrix} \boldsymbol{u} \\ \boldsymbol{\varphi} \end{bmatrix}=\begin{bmatrix} \boldsymbol{F}_1 \\ \boldsymbol{F}_2 \end{bmatrix} \tag{15}$$

where, $\boldsymbol{u}$ and $\boldsymbol{\varphi}$ are velocity and concentration degrees of freedom, respectively. The system matrices $\boldsymbol{M}$, $\boldsymbol{K}$, $\boldsymbol{D}^{\varphi}$ and $\boldsymbol{K}^{\varphi}$ are assembled following a standard finite element methodology. Matrices $\boldsymbol{D}^{U\varphi}$ and $\boldsymbol{K}^{U\varphi}$ represent the coupled effect attribute. COMSOL has solved these nonlinear equations using CG solver based on AMG.

4. MACROMODEL EXTRACTION FOR MICROMIXER

The COMSOL software was used to conduct finite element simulation for the micromixer and some characteristic parameters are set up and presented in Table 1.

Table 1. Finite element simulation parameters

Simulation parameter	*Value*
Density of fluid	10^3 *(kg/m^3)*
Dynamic viscosity of the fluid	1.002×10^{-3} *(Pa·s)*
Diffusion coefficient	10^{-10} *(m^2/s)*
Channel width	3×10^{-4} *(μm)*
Wall boundary	*No slip*
1 input concentration	*0.01 (mol/m^3)*
2 input concentration	*0.1 (mol/m^3)*

The command "assemble" can extract stiffness matrix and other system matrices from COMSOL finite element model analysis outputs, and the command code is:

$$[\,\boldsymbol{K},\boldsymbol{L},\boldsymbol{M},\boldsymbol{N}\,] = assemble(\ fem\ ); spy(\ \boldsymbol{K}\ ) \quad (16)$$

Using the system matrices extracted from the finite element model, Lanczos algorithm is executed in MATLAB language for the steady-state analysis of the micromixer. We reduced the original model to *40* and *20* order in MATLAB language and we also calculated the macromodel output value. The calculation times of COMSOL, *40* order macromodel and *20* order macromodel are *2.2 s*, *0.027 s* and *0.021* s, respectively. The macromodel is two orders of magnitude faster than the finite element model. The micromixer output concentration results from COMSOL, *40* and *20* order macromodel are shown in Figure 4. As it can be seen from Figure 4, the calculation error from *40* order model is less *5%* less than the one obtained by COMSOL, therefore, it can be concluded that the calculation error decreases along with the order number increment. Furthermore, it means that the compromise between calculation precision and speed should be taken into consideration.

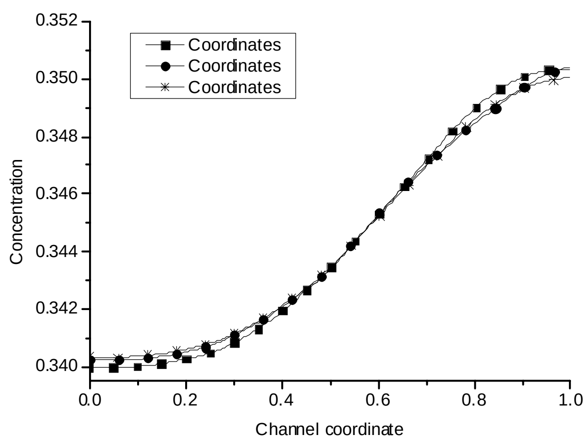

Fig. 4 COMSOL model, 40 order macromodel and 20 order macromodel output concentration results

5. CONCLUSIONS

A macromodel is presented and successfully calculated for the microfluidic chip micromixer. It has been proved that the macromodel based on Kyle subspace is an effective method for the MEMS simulation. The strongly coupled nonlinear microfluidic problems can be solved by the use of the macromodel method in combination with the finite element analysis. In the future, the macromodel method based on Kyle subspace will have a great potential in the design and simulation of microfluidic analysis systems.

6. ACKNOWLEDGMENTS

The authors are grateful to Liaoning Province Key Laboratory Funded Projects (No: LS2010080, LKF2011020), and National Science Technology Support Plan Projects (No: 2012BAF12B08-5).

7. REFERENCES

[1] J. Cao, P. Cheng and F.J. Hong, A numerical study of an electrothermal vortex enhanced micromixer, *Microfluidics and Nanofluidics*, Vol. 5, No. 1, pp. 13-21, 2008.

[2] C.A. Cortes-Quiroz, M. Zangeneh and A. Goto, On multi-objective optimization of geometry of staggered herringbone micromixer, *Microfluidics and Nanofluidics*, Vol. 7, No. 1, pp. 29-43, 2009.

[3] W. Dai and Y. P. Zhao, The nonlinear phenomena of thin polydimethylsiloxane (PDMS) films in electrowetting, *International Journal of Nonlinear Sciences and Numerical Simulation* Vol. 8, No. 4, pp. 519-526, 2007.

[4] O.-T. Son, J.W. Roh, S.-H. Song, J.-S. Park, W. Lee and H.-I. Jung, Continuous micro-magnetophoretic separation using a dipole magnetic field, *BioChip Journal*, Vol. 2, No. 3, pp. 186-191, 2008.

[5] Y.-Q. Wan, Q. Guo and N. Pan, Thermo-electro-hydrodynamic model for electrospinning process, *International Journal of Nonlinear Sciences and Numerical Simulation*, Vol. 5, No. 1, pp. 5-8, 2004.

[6] Y.C. Zeng, Y. Wu, Z.G. Pei and C.W. Yu, Numerical approach to electrospinning, *International Journal of Nonlinear Sciences and Numerical Simulation*, Vol. 7, No. 4, pp. 385-388, 2006.

[7] D.H. Shou and J.H. He, Application of parameter-expanding method to strongly nonlinear oscillators, *International Journal of Nonlinear Sciences and Numerical Simulation*, Vol. 8, No. 1, pp. 121-124, 2007.

[8] Y. Wang, Q. Lin and T. Mukherjee, A model for Joule heating-induced dispersion in microchip electrophoresis, *Lab on a Chip*, Vol. 4, No. 6, pp. 625-631, 2004.

[9] D. Vasilyev, M. Rewienski and J. White, Macromodel generation for bioMEMS components using a stabilized balanced truncation plus trajectory piecewise-linear approach, *IEEE Transactions on Computer-Aided Design of Integrated Circuits and Systems*, Vol. 25, No. 2, pp. 285-293, 2006.

[10] H.M. Park and J.Y. Lim, A reduced-order model of the low-voltage cascade electroosmotic micropump, *Microfluidics and Nanofluidics*, Vol. 6, No. 4, pp. 509-520, 2009.

[11] R. Qiao and N.R. Aluru, A compact model for electroosmotic flows in microfluidic devices, *Journal of Micromechanics and Microengineering*, Vol. 12, No. 5, pp. 625-635, 2002.

[12] X. He and S. Hauan, Microfluidic modeling and design for continuous flow in electrokinetic mixing-reaction channels, *Aiche Journal*, Vol. 52, No. 11, pp. 3842-3851, 2006.

[13] M. Troyer, H. Tsunetsugu and D. Wurtz, Thermodynamics and spin gap of the Heisenberg ladder calculated by the look-ahead Lanczos-algorithm, *Physical Review B*, Vol. 50, No. 18, pp. 13515-13527, 1994.

[14] S. Sundar and B.K. Bhagavan, Comparison of Krylov subspace methods with preconditioning techniques for solving boundary value problems, *Computers & Mathematics with Applications*, Vo. 38, No.11-12, pp. 197-206, 1999.

[15] T.J. Frankcombe and S.C. Smith, Fast, scalable master equation solution algorithms, IV. Lanczos iteration with diffusion approximation preconditioned iterative inversion, *Journal of Chemical Physics*, Vol. 119, No. 24, pp. 12741-12748, 2003.

PRIKAZ NELINEARNOG MAKROMODELA TEMELJENOG NA KRYLOVLJEVOM POTPROSTORU PRIKLADNOG ZA SIMULACIJU RADA MIKROMIKSERA MIKROFLUIDNOG PROCESORA

SAŽETAK

U ovome se radu polazi od pretpostavke da konvencionalne metode numeričke analize nisu dostatne za simulaciju mikro-elektro-mehaničkog-sustava (MEMS) koji sadrži polje fluida. Međutim, korištenjem makromodela s primjenom nelinearne analize mogu se simulirati karakteristike mikro-polja toka. U ovome su radu prikazane postavke makromodela mikromiksera mikrofluidnog procesora pri čemu je korištena Krylovljeva metoda projiciranja potprostora. Funkcije sustava dobivene su metodom konačnih elemenata uz korištenje softvera COMSOL. Za diskretizirani model mikromiksera uzeta je analiza polja koncentracije. Red funkcije konačnih elemenata reduciran je pomoću Krylovljeve metode projekcije potprostora drugog reda bazirane na Lanczosovom algoritmu. Pokazano je da se rezultati dobiveni korištenjem makromodela podudaraju s rezultatima dobivenim analizom s primjenom konačnih elemenata, s tim da je vrijeme trajanja simulacije pri korištenju makromodela stotinu puta kraće od vremena trajanja simulacije korištenjem metode konačnih elemenata. U praktičnoj primjeni, ovaj bi makromodel trebao olakšati dizajniranje mikrofluidnih naprava sa sofisticiranom mrežom kanala.

Ključne riječi: *makromodel, Krylovljev potprostor, mikromikser, mikro-elektro-mehanički sustavi (MEMS).*