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ANALYZING MICRO-ELECTRO-MECHANICAL-FLUIDIC SYSTEMS BY 2D COUPLED-FIELD ANALYSES

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Abstract. *The major technical barrier in developing new microdevices lies in the lack of understanding physical phenomena and their interactions that occur in multiphysical microsystems. Most of them rely on interactions of thermal, mechanical, electric, magnetic and/or fluidic fields for performing their intended functions. So, to make a step in advance, it is not enough to understand these areas individually, but the coupled effects of these phenomena at the same time. This is possible by using coupled-field analyses that take into account interactions between two or more different disciplines of engineering. The typical representative is an analysis of the piezoelectric micropump as an electric-structure-fluid coupled microsystem. Theoretical considerations and the procedure of modeling a piezoelectric micropump as a multidisciplinary microsystem with coupled-field effects by 2D coupled-field analyses of the simulation software ANSYS will be shown in this paper.*

Key Words: *Microsystems, Modeling, Physical Effects, Coupled-field Analysis*

1. INTRODUCTION

The rapid progress in microsystems technology and in developing new, complex microdevices is intensely supported by a modern concept of designing new devices that substitute the traditional way based on experimental investigations that involved several design and fabrication cycles until the optimal specifications were satisfied. That new concept is based on Computer Aided Design (CAD) with different numerical simulation tools that are an essential key for designing and manufacturing Micro-Electro-Mechanical-Systems (MEMS) with higher performance and reliability, reduced costs, shorter development cycles and a time-saving approach.

Though the concept of MEMS has been known for more than 20 years, the commercialization of microsystem technology has not progressed as fast as Integrated Circuit (IC) chip technology. The major technical barrier in developing new, revolutionary microdevices that have potential applications in medical, environmental, military and industrial

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applications, lies in the lack of understanding of physical phenomena and their interactions that occur in multiphysical microsystems. Most microdevices rely on interactions of thermal, mechanical, electric, magnetic and/or fluidic fields for performing their intended functions. So, to make a step in advance it is not enough to understand these areas individually, but the coupled effects of these phenomena at the same time. For that purpose CAD with numerical simulation tools have been developed to model and simulate microsystems including interactions between different physical fields by coupled-field analyses.

A coupled-field analysis is an analysis that takes into account the interaction between two or more different disciplines of engineering. For example, a piezoelectric analysis at a piezoelectric actuator handles the interaction between structural and electric fields. Other examples of coupled-field analyses are thermal-stress analyses for bimetallic actuators, magneto-structural analyses for electromagnetic actuators, fluid-structure analyses for fluid flow considerations and finally problems that at the same time involve complex interactions of thermal, structural and electrical fields with the flow field. The last example is the most complex analysis of microsystems and its representative is an analysis of a piezoelectric micropump as an electric-structure-fluid coupled microsystem.

Currently, there are many types of micropumps used for variety of purposes. But they are mainly applied as drop-on-demand micropumps. This means that a micropump, under an electric signal given by a driving system, can eject high-speed droplets out of the nozzle with tens microns of diameter in a few microseconds. Due to high reliability, high stability, long life, high firing speed and the applicability for many kinds of liquid, the piezoelectric micropumps provide much potential for variety of applications. These advantages - together with ejecting precise and uniform droplets, accurate placing of droplets on specified positions, different operating conditions, batch microfabrication and so on - are the reason to take, as the subject of this paper, the modeling of a piezoelectric micropump as a multidisciplinary micro-electro-mechanical-fluidic-system with coupled-field effects.

2. Piezoelectric Micropumps

In order to understand the working principle of a typical piezoelectric micropump during which high pressure on the fluid in the chamber is generated, in order to eject droplets out of the nozzle on the bases of deformations (radial shrinkage, bend, extension or shear) of a piezoelectric material under a high electric field and interaction of a silicon membrane and a working fluid across the fluid-structure interface, a cross-sectional view of the piezoelectric micropump is displayed in Figure 1.

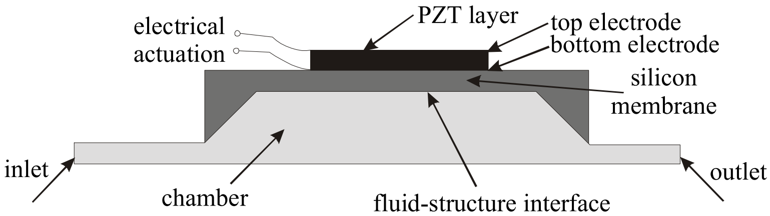

Fig. 1. A Cross-sectional View of Piezoelectric Micropump

The piezoelectric micropump has a piezoelectric ceramic (PZT) bonded on the outside of a membrane. The membrane forms a chamber that is filled with the working fluid and which is made together with an outlet nozzle and an inlet feeding channel in a silicon wafer by wet etching. There are top and bottom electrodes on the PZT layer connected to the driving system for electrical actuation. Application of a high voltage electric impuls bends the PZT layer. This causes the membrane to move downward which decreases the chamber volume while a high pressure in the liquid inside the chamber is formed. Then the pressure forces some liquid from the chamber to move back into the feeding channel and the rest, that is, the major part of the liquid is forced to move out from the nozzle in the form of a droplet. During this process the pressure also resists the membrane motion and tends to slow down the deformation. Once the membrane reaches the lowest point, the inertial energy transforms into internal elastic energy, which causes the membrane to rebound and move upwards. Finally, the upward motion increases the chamber volume and sucks some liquid back from the nozzle and the rest from the feeding channel. After that the piezoelectric micropump is ready for another electric impulse and another working cycle.

2D COUPLED-FIELD ANALYSES OF A PIEZOELECTRIC MICROPUMP

As mentioned above, it can be concluded that the working principle of the piezoelectric micropump is a very complicated process with the coupling of piezoelectricity, elasticity and multiphase flow of immiscible fluids (liquid and gas) with the surface tension on their free contact surface. For analyzing such complex coupled-field problems in two dimensions the software package ANSYS is a very good CAD tool based on FEA (Finite Element Analysis) that can handle coupled-field analyses.

In this package the procedure for a coupled-field analysis depends on the choice of fields to be coupled. According to the described working principle of the piezoelectric micropump, the first interaction, typical for the actuating piezoelectric ceramic, corresponds to the deformations of a piezoelectric material under the input electric field. Therefore, as a first step in the modeling procedure, the relations existing between electrical and structural physical fields in the PLZ layer are coupled. In ANSYS this is done by the direct coupling method. This method usually involves just one analysis that uses a coupled-field element type, especially made for the concrete coupling purpose, containing all necessary degrees of freedom. In the mentioned case of piezoelectric coupling PLANE13 – 2D coupled-field solid element is utilized. It has a 2D magnetic, thermal, electrical, piezoelectric and structural field capability with limited coupling between the fields. It has four nodes and for a piezoelectric analysis by KEYOPT(1) = 7 UX, UY and VOLT degrees of freedom are defined per node. KEYOPT(3) = 2 defines the usage of this element with the plane stress option.

The piezoelectric coupling [1] is handled by calculating element matrices or element load vectors that contain all necessary terms according to the electromechanical constitutive equations for linear material behavior:

$$\begin{Bmatrix} \{T\} \\ \{D\} \end{Bmatrix} = \begin{bmatrix} [c] & [e] \\ [c]^T & -[\varepsilon] \end{bmatrix} \begin{Bmatrix} \{S\} \\ -\{E\} \end{Bmatrix} \tag{1}$$

where:

$\{T\}$ = stress vector (referred to as σ);
$\{D\}$ = electric flux density vector;
$\{S\}$ = strain vector (referred to as ε);
$\{E\}$ = electric field vector;
$[c]$ = elasticity matrix (evaluated at constant electric field (referred to as $[D]$));
$[e]$ = piezoelectric stress matrix;
$[\varepsilon]$ = dielectric matrix (evaluated at constant mechanical strain).

Equation (1) is derived from the usual constitutive equations for structural and electrical fields, respectively, involving the coupling terms - the piezoelectric matrix $[e]$. The finite element discretization is performed by establishing nodal solution variables and element shape functions over an element domain, which approximates the solution. This direct coupling solution is advantageous when the coupled-field interaction is highly nonlinear and is best solved in a single step using the existing coupled formulation.

The piezoelectric material displacements, induced in this way, are then applied to the structural membrane that further acts on the fluid in the chamber. But, at the same time, the fluid has damping effects on the membrane, so that the nonlinear transient Fluid-Structure Interaction (FSI) is the next coupled-field problem that must be taken into account. This is necessary because transfer of fluid forces from the fluid to the structure and displacements and velocities from the structure to the fluid occurs simultaneously across the fluid-solid interface. In this case for the modeling purposes in ANSYS the fluid-solid sequential coupling analysis is predicted. It provides a fluid-solid interaction between finite elements in the fluid and structural region. Figure 2 shows the algorithm of the fluid-solid sequential coupling analysis. From the algorithm it can be seen that the equations for the fluid and solid domains are solved sequentially and fluid forces and heat fluxes and solid displacements, velocities, and temperatures transfer between the fluid and solid regions across the fluid-solid interface, with the fluid mesh updating between sequential time steps. The algorithm continues to loop through the solid and fluid analyses until convergence is reached for that time step. Convergence in the stagger loop is based on the quantities being transferred at the fluid-solid interface.

To perform a fluid-solid interaction analysis, the fluid model and the finite element mesh for the fluid region are created firstly. Then the appropriate boundary conditions for the fluid region and material properties for the fluid analysis are applied. The model is then ready for solution in ANSYS/FLOTRAN as a CFD (Computational Fluid Dynamics) product that offers comprehensive tools for analyzing two- and three-dimensional fluid flow fields. FLUID141 – 2D Fluid element with four nodes is used for modeling the transient state of a single phase fluid system in two-dimensional analyses. For this element, the velocities are obtained from the conservation of momentum principle, and the pressure is obtained from the conservation of mass principle. For using FLUID141 in a fluid-solid interaction analysis, as in this case, KEYOPT(4)=1 allows displacement DOFs (UX and UY) to specify motion of boundaries.

In the case of moving boundaries the equations of motion can be based on an Eulerian (fixed) frame of reference. The governing equations may also be formulated in a Lagrangian frame of reference, i.e. the reference frame moves with the fluid particles. Both the formulations have their advantages and disadvantages. With the Eulerian framework it is not straightforward to solve problems involving moving boundaries or deforming domains. While such problems are more suitable for a Lagrangian framework, in practice the mesh distortions can be quite severe leading to mesh entanglement and other inaccuracies. A pragmatic way around this problem is to move the mesh independently of the fluid particles in such a way as to minimize the distortions. This is the Arbitrary Lagrangian Eulerian (ALE) formulation [2], which involves moving the mesh nodal points in some heuristic fashion so as to track the boundary motion/domain deformation and at the same time minimize the mesh degradation.

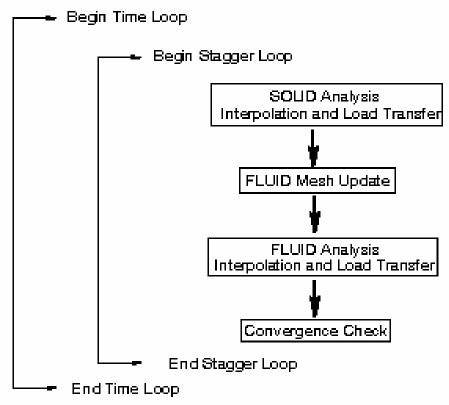

Fig. 2. Fluid-solid Sequential Coupling Algorithm for the Time and Stagger Loops

The ALE formulation for describing the fluid flow in the fluid domain for FSI problems can be written for the equation of momentum as:

$$\rho_F\left(\frac{\partial \vec{v}}{\partial t} + \vec{v}\cdot\nabla\vec{v}\right) - \nabla\cdot\sigma_F = \vec{f}_F \tag{2}$$

and for the equation of continuity:

$$\nabla\cdot\vec{v} = 0\,, \tag{3}$$

where $\vec{v}$ is the fluid velocity vector; ρ_F is the fluid mass density; σ_F is the total fluid stress tensor and $\vec{f}_F$ is the applied body force vector in the fluid domain.

The solid model and the finite element mesh for the solid region follow in a fluid-solid analysis together with the appropriate boundary conditions for the solid region, material properties for the solid analysis, and the appropriate solution options for a structural analysis. PLANE42 – 2D Structural. The solid element is used for two dimensional modeling of solid structures. With the option KEYOPT(3) = 0 this element can be used as an element with plane stress state. Four nodes having two degrees of freedom at each node define this element: translations in the nodal x and y directions.

The transient dynamic analysis (sometimes called time-history analysis) is a technique used in ANSYS to determine time-varying displacements, strains, stresses, and forces in the structure as the dynamic response of the membrane structure under the action of the time-dependent fluid forces from the fluid region. The basic equation of motion solved by the transient dynamic analysis can be expressed according to the equation of momentum in the structural domain:

$$\rho_S \frac{\partial^2 \vec{u}}{\partial t^2} - \nabla \cdot \sigma_S = \vec{f}_S \,, \tag{4}$$

where ρ_S is the density of the structural material, $\vec{u}$ is the displacement, σ_S is the stress tensor for the elastic structural material and $\vec{f}_S$ is the applied body force in the structural domain.

The coupling conditions for the interface between the fluid and the solid region are kinematic and equilibrium conditions. The kinematic condition is a no-slip condition, i.e., continuity in velocity expressed as:

$$\vec{v}_i = \dot{\vec{u}}_i \,, \tag{5}$$

and the equilibrium condition is interface continuity in tractions replaced by continuity of stresses written as:

$$\sigma_{ij}^S n_j^S + \sigma_{ij}^F n_j^F = 0 \,, \tag{6}$$

where n_j^S is the outward unit normal to the solid at the interface between solid and fluid in the deformed configuration, so as $n_j^S = -n_j^F$ (indexes i and j define directions of components according to axes of the applied 2D coordinate system).

These equations are expressed in terms of partial differential equations that are discretized with a finite element based technique to be used in the numerical solving procedures.

Besides taking into account classical coupled-field effects in a micropump modeling, an additional very important problem in the simulation of the multiphase fluid flow is to track the free contact surface between the immiscible fluids which have quite a large difference in the densities. In the case of a micropump the first fluid is a liquid that is inside the pump and the second fluid is a gas (the air) outside the pump. Due to a low density, the inertia of the gas is usually negligible, so the only influence of the gas is the pressure exerted on the interface. Hence, the region of gas need not be modeled, and the free surface is simply modeled as a boundary with constant pressure. Taken into account together with the surface tension on the free contact surface, it becomes very important to find optimal parameters for making droplets from the fluid that comes out of the nozzle of the micropump. The fluid that comes out of the nozzle need not be in the form of a droplet. It may also leak or make jets. Therefore, only with optimal parameters for fluid pressure, velocity, density, viscosity, surface tension coefficient and geometrical forms and dimensions of the chamber and nozzle can the intention of making droplets be satisfied.

As a numerical method for the multiphase fluid flow analyzing the fractional Volume Of Fluid (VOF) method has been developed to determine the shape and track the location of the free contact surface of the immiscible fluids. For a VOF analysis in ANSYS/FLOTRAN an advection algorithm for the volume fraction (VFRC) to track the evolution of the free surface is used. The VFRC value for each element varies from zero to one, where zero denotes an empty element containing no fluid (only gas) and one denotes a full element thoroughly occupied by the fluid. The values between zero and one indicate that the corresponding elements are partially full or surface elements (henceforth called partial elements), and the free surface can thus be determined by the distribution of the VFRC field.

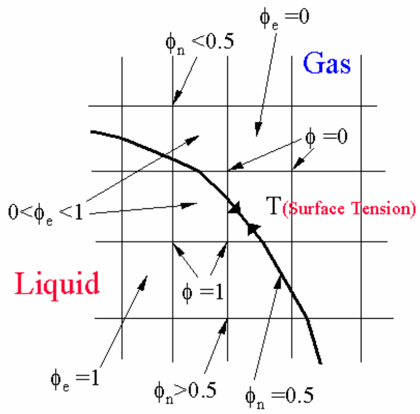

Fig. 3. Representation of the VOF Method with the Free Contact Surface of Immiscible Fluids

Figure 3 shows the representation of this method based on the concept of the fractional volume of fluid with the position of the free contact surface of immiscible fluids. ϕ_e is the volume fraction of fluid within an element. $\phi_e = 1$ means the element is full of liquid. $\phi_e = 0$ means full of gas (or other immiscible fluid). When $0 < \phi_e < 1$, the element contains ϕ_e fraction of liquid and $1-\phi_e$ fraction of gas. The nodal volume fraction of fluid ϕ_n is defined by averaging ϕ_e of the surrounding elements. Under such circumstance, the motion of the free contact surface is determined by the evolution of ϕ_e. From the law of mass conservation, the volume fraction of fluid F is governed by the following equation:

$$\frac{\partial F}{\partial t} + \vec{u} \cdot \nabla F = 0\,, \tag{7}$$

where $\vec{u}$ is the velocity component.

In order to study complex flow problems, different VOF algorithms have been developed that are applicable to the unstructured mesh. In ANSYS/FLOTRAN, the VOF algorithm first computes the motion of the polygon of fluid in a Lagrangian sense and then utilizes the computational geometry of the intersection of two polygons to determine the VFRC fluxes. This method is referred to as the Computational Lagrangian-Eulerian Advection Remap (CLEAR) method [3]. This CLEAR- VOF method tracks the free surface explicitly in time, and it is, therefore, necessary that the transient solution option for a VOF analysis should be used. Currently in ANSYS/FLOTRAN, VOF capability is available only for quadrilateral elements for two dimensional planar or axisymmetric analyses. In the case of micropumps analyzing this means that only two dimensional models can be taken into consideration. For a VOF analysis, boundary conditions are required for boundary nodes that belong to at least one non-empty (partial or full) element.

It has been said that for the dynamic behavior at the interface between a gas and liquid the surface tension on the free contact surface, as an inherent characteristic of material interfaces, must be also taken into account in the multiphase fluid flow analysis.

In ANSYS/FLOTRAN, the surface tension is modeled through a Continuum-Surface Force (CSF) method [4]. This is based on the fact that a surface force with two components represents the surface tension. The first component is normal to the free contact surface due to the local curvature, and the second one is tangential to the free contact surface due to local variations of the surface tension coefficient. Then, thus obtained surface force is reformulated into an equivalent continuous volumetric force in the momentum equation that acts on the fluid elements everywhere within a thin transition region near the interface with the gas phase.

The surface tension is a force per unit area given by:

$$\vec{f}_S = \sigma\kappa\hat{n} + \nabla_{\hat{t}}\sigma \,, \tag{8}$$

where is σ the surface tension coefficient, $\vec{n}$ the unit normal vector in the following form:

$$\hat{n} = \frac{\vec{n}}{|\vec{n}|} = \frac{\nabla F}{|\nabla F|} \,, \tag{9}$$

then κ the surface curvature:

$$\kappa = -\nabla \cdot \hat{n} = \frac{1}{|\vec{n}|}\left[\left(\frac{\vec{n}}{|\vec{n}|} \cdot \nabla\right)|\vec{n}| - (\nabla \cdot \vec{n})\right] \tag{10}$$

and $\nabla_{\hat{t}}$ the surface gradient that is given in the function of the unit tangent vector at the surface $\hat{t}$:

$$\nabla_{\hat{t}} = \hat{t}(\hat{t} \cdot \nabla) \,. \tag{11}$$

In Equation (8), the first term is acting normal to the interface, and is directed toward the center of the local curvature of the interface. The second term is acting tangential to the interface, and is directed toward the region of higher surface tension coefficient *σ*.

After defining the surface force, in the CSF method, it is reformulated by the Gauss' theorem into the volumetric force $\vec{F}_S$ as follows:

$$\vec{F}_S = \vec{f}_s \delta_s \frac{F}{< F >} \,, \tag{12}$$

where *F* is a volume fraction , <*F*> the averaged volume fraction across the interface and δ_s the surface delta function according to the following:

$$\delta_s = |\vec{n}| = |\nabla F| \,. \tag{13}$$

Function δ_s has non-zero value only within a finite thickness transition region near the interface, and corresponding volumetric force $\vec{F}_S$ only acts within this transition region.

The last term that is necessary for fluid flow analyzing is wall static contact angle θ_w that describes the effect of wall adhesion at the solid boundary. It is defined as the angle between the tangent to the fluid interface and the tangent to the wall. The angle is not only a material property of the fluid but also depends on the local conditions of both the fluid and the wall. Its input is a constant value between 0° and 180°. The wall adhesion force is then calculated in the same manner as the surface tension volume force [4] using Equation (8) except that the unit normal vector at the wall is modified as follows:

$$\vec{n} = \hat{n}_z \cos\theta_z + \hat{t}_z \sin\theta_z \, , \tag{14}$$

where $\hat{n}_z$ is the unit wall normal vector directed into the wall and $\hat{t}_z$ is the unit vector normal to the interface near the wall.

CONCLUSION

Theoretical systematization and the modeling procedure for the complex simulation of the piezoelectric micropump with the coupling of piezoelectricity, elasticity and multiphase flow of immiscible fluids with surface tension on their contact surfaces was presented for planar models in the simulation package ANSYS by coupled-field analyses. They can be further used for obtaining validated physically-based models of different types of piezoelectric micropumps as multidisciplinary microsystems that could be reliably used for designing new piezoelectric micropumps, as well as for giving useful hints and instructions in solving important development questions: optimal geometrical parameters, nozzle shape, applied voltage, fluid loss, refill time, immunity on temperature variations, droplet velocity, secondary droplets forming and other characteristics, for quickly and efficiently satisfying different working demands and tasks.

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ANALIZA MIKRO-ELEKTRO-MEHANIČKO-FLUIDNIH SISTEMA PRIMENOM 2D UPARENIH ANALIZA

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Glavna tehnička barijera u razvoju novih mikrouređaja leži u činjenici da je veoma teško shvatiti fizičke pojave, a naročito njihove uzajamne interakcije koje egzistiraju u multifizičkim mikrosistemima. To je posledica toga što se ispunjenje karakterističnih funkcija kod većine mikrokomponenata zasniva na složenim međusobnim uticajima toplotnog, mehaničkog, električnog, magnetnog i/ili fluidnog fizičkog polja. Zbog toga nije dovoljno da se poznaju individualni procesi unutar ovih oblasti, već je potrebno da se shvate efekti ovih fenomena pri njihovoj međusobnoj interakciji. Takvi efekti nazivaju se upareni efekti i u cilju njihove analize razvijene su takozvane uparene analize pomoću kojih se analiziraju međusobne interakcije multifiičkih efekta koji potiču iz dve ili više različitih fizičkih disciplina. Karakterističan primer je analiza piezoelektrične mikropumpe sa istovremenom interakcijom veličina iz električne, mehaničke i fluidne oblasti. U ovom radu će biti prikazani teorijska razmatranja i procedura za modeliranje piezoelektrične mikropumpe kao jednog multidisciplinarnog mikrosistema pomoću 2D uparenih analiza u softverskom paketu ANSYS.

Ključne reči: *Mikrosistemi, modeliranje, fizički efekti, uparena analiza.*