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# Implementation of General Coupling Model of Electromigration in ANSYS

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**Abstract**— In this paper, a recently developed theory – general coupling model of electromigration, is implemented in ANSYS. We first identify several errors provided in ANSYS manuals for electromigration modeling. Then the general coupling model is implemented in ANSYS and the detailed description is presented. Finally, a 1-D confined metal line with a perfectly blocking condition is presented as a benchmark problem, in which the finite element solutions are in excellent agreement with the analytical solutions.

**Keywords**—electromigration; general coupling theory; multi-physics modeling; finite element analysis.

## I. INTRODUCTION

Electromigration remains as one of the critical reliability issues at both device and package levels as the current density is increasingly higher due to the continuous scaling down of interconnect technology [1-3]. Essentially, electromigration is an enhanced mass transport process driven by high electrical current density, which, over time, causes void nucleation near the cathode side and hillock development near the anode side, resulting in opens and shorts in microelectronic devices [4, 5].

While the mass transport of electromigration is induced by electron wind force, it is not the only driving forces at work. A series of works done by Blech from 1976 showed that in addition to electromigration also stress-migration in the opposite direction takes place [6-8] and this driving force is induced by the gradient of mechanical hydrostatic stress. Kirchheim *et al.* [9,10] further derived the equations of vacancy transport and stress development considering the vacancy generation and annihilation. And, the work done by Korhonen [11] proposed a model to couple the stress evolution with vacancy transport, which was later used in the electromigration simulation software MIT/Emsim [12], developed by the group of Thompson. However, for both Kirchheim's and Korhonen's models, the self-diffusion (concentration gradient) in electromigration analysis is neglected, and an over-simplified assumption was used to obtain the coupling relationship of stress and vacancy concentration.

Sarychev and Zhinikov [13] proposed another physical model to couple the stress evolution with the vacancy transport, and a sophisticated constitutive model was established. Then, Lin and Basaran implemented this model in a general finite element (FE) procedure and studied the electromigration in pure metal line and solder joint [14,15].

However, the numerical results in Sarychev's study and Lin's FE simulations were not available to compare with any numerical results published before. Furthermore, Sukharev *et al.* also developed a multi-physics model and implemented it in a general commercial FE software [16]. Except above mentioned works, there are many papers with detailed numerical analysis and results, but some of the coupling terms in those governing equations are missing in one way or another. [17-24]. Until recently, a general coupling theory for electromigration has been developed, in which all important physical fields and its effects on electromigration are considered and fully coupled. One-dimensional (1-D) numerical results have been presented and compared to the literature [25]. Nevertheless, the implementation of such a general coupling theory for three-dimensional analysis, particularly in commercial finite element software, is to be developed.

In this paper, the implementation of the general coupling model of electromigration using ANSYS is presented. We first review the current practice of electromigration modeling in ANSYS, including those tested case studies provided in ANSYS verification manual, ANSYS online manual and the paper published by ANSYS. Then, we will introduce the general coupling model and implement it in finite element analysis by using the current capability of ANSYS multi-physics modeling, based on some approximations. Finally, a 1-D confined metal line with a perfectly blocking condition is presented as a benchmark problem to demonstrate how the modeling can be conducted with accuracy in ANSYS.

## II. CURRENT PRACTICE OF ELECTROMIGRATION MODELING IN ANSYS

### A. Tested Case in ANSYS Verification Manual

In the test case (VM220) shown in ANSYS verification manual, the diffusion and mass transport due to electromigration is presented by using: a constant current loading on a rectangular conductor with length  $L$  and height  $H$ . At one end of the conductor ( $x=-L$ ), a constant vacancy concentration is set as boundary condition. At the other end of conductor ( $x=0$ ), a zero-flux boundary condition (blocking diffusion barrier) is applied. To solve this electromigration problem, two approaches are provided in VM220.

The first approach considers the electromigration as a simple diffusion problem, using the diffusion element (PLANE238) and applying the electron wind force as a body load of transport velocity. The second approach uses a coupled electric-diffusion element (PLANE223) with KEYOPT(1)=100001. In both cases, the effects of mechanical stress and temperature gradient are neglected

and the sink/source term is set as “0”. As a result, two approaches give the same but incorrect results. As a matter of fact, it has been long recognized [26] that without considering sink/source term and the effect of stress-migration, the time to reach the steady-state for electromigration process is only ~1 second, which is not supported by experimental data. This means that the tested case VM220 selected an incorrect electromigration model for the verification study.

### B. Cases Studies in ANSYS Online Manual

In ANSYS Mechanical APDL 19.1 Online Manual, two additional examples of electromigration modeling are demonstrated in the “Coupled-Field Analysis Guide”, to show its capability to simultaneously model electromigration, stress-migration, and thermo-migration induced by current loading as well as mechanical and thermal stresses.

Example 1: Transient stress build-up due to electromigration. ([https://ansyshelp.ansys.com/account/secured?returnurl=/Views/Secured/corp/v191/ans\\_cou/coupsttheldiff.html](https://ansyshelp.ansys.com/account/secured?returnurl=/Views/Secured/corp/v191/ans_cou/coupsttheldiff.html)). In this example, a constant current loading is applied on a metal line with blocking diffusion condition at both ends. The temperature of the conductor keeps constant. The coupled field element SOLID226 with KEYOPT(1)=100111 is selected to simultaneously consider the electrical, structural, thermal and diffusion fields. However, there are several errors in this example:

1. The sink/source term is set as “0” in the vacancy transport equation. The study done by Shatzkes and Lloyd has shown that the absence of sink/source term can cause the predicted lifetime of electromigration in a very short time scale. To avoid this problem, this example incorrectly adjusts the diffusivity to 10% of its normal value. As a result, the velocity of vacancy migration is decreased and the time to reach steady state of electromigration is extended. However, for the steady-state results, the obtained maximum hydrostatic stress is only ~8 MPa that is too small to compare with any numerical results published in literature.

2. The values of the vacancy relaxation factor and the coefficient of diffusion strain shown in APDL file are given without any basis or literature support. This example attempts to obtain the “reasonable” numerical results by manipulating some material properties that do not exist.

3. And, the mechanical boundary condition shown in APDL file is set as fully fixed at each node in metal line:

```
d, all, ux, 0
d, all, uy, 0
d, all, uz, 0
```

This is not a correct boundary condition setting. It literally reads that each point anywhere is fixed during electromigration. When the electrical current passes through the metal line, the electron wind force causes atomic transport along the electron direction, which can induce displacement along the length of the line.

Example 2: Electromigration and stress migration in a solder joint. ([https://ansyshelp.ansys.com/account/secured?returnurl=/Views/Secured/corp/v191/ans\\_cou/coupstelecdiff.html?q=migration model](https://ansyshelp.ansys.com/account/secured?returnurl=/Views/Secured/corp/v191/ans_cou/coupstelecdiff.html?q=migration%20model)). In this example, a half symmetry model of a SnAgCu (SAC) solder joint sandwiched between two copper plates is studied. The model is meshed with the SOLID227 coupled-field element with KEYOPT(1) = 100101. A constant current load goes through the solder from the bottom plate to the top plate. The uniform temperature of 200 °C is set to the solder ball. Although this example provides a complete process in modeling electromigration in solder, three errors pointed previously in Example 1 are also presented in this example.

### C. Electromigration Modeling using ANSYS by [27]

The developers at ANSYS published a paper [27] for electromigration modeling, which provides additional information of the theory and the implementation in ANSYS using R18.1. For electromigration, the total vacancy flux is written as follows,

$$\mathbf{J}_v = -D_v \nabla \bar{C}_v + \frac{D_v \bar{C}_v Z^* e}{kT} \mathbf{E} - \frac{D_v \bar{C}_v \Omega}{kT} \nabla \sigma + \frac{D_v \bar{C}_v Q^*}{kT^2} \nabla T \quad (1)$$

where  $D_v$  is the vacancy diffusivity ( $\text{m}^2/\text{s}$ ),  $\bar{C}_v$  is the normalized vacancy concentration ( $\text{m}^{-3}$ ),  $Z^*$  is the effective charge number ( $Z^* > 0$ ),  $e$  is the elementary charge (C),  $\mathbf{E}$  is the electrical field (V/m),  $k$  is the Boltzmann’s constant,  $T$  is the absolute temperature (K),  $\Omega$  is the atomic volume ( $\text{m}^3$ ),  $Q^*$  is the heat of vacancy transport (kJ/mol) ( $Q^* > 0$ ), and  $\sigma$  is the hydrostatic stress.

The governing equation of vacancy transport is written as follows,

$$\frac{\partial \bar{C}_v}{\partial t} + \nabla \cdot \mathbf{J}_v = G \quad (2)$$

where  $G(\bar{C}_v)$  is the rate of vacancy generation/annihilation per unit volume that can be used to define the sink/source term. Applying Eq. (1) to the Eq. (2) and omitting G term, we can obtain the following governing equation,

$$\frac{\partial \bar{C}_v}{\partial t} = -D_v \nabla \cdot (-\nabla \bar{C}_v + \frac{Z^* e \mathbf{E} \bar{C}_v}{kT} - \frac{\Omega}{kT} \bar{C}_v \nabla \sigma + \frac{Q^*}{kT^2} \bar{C}_v \nabla T) \quad (3)$$

In ANSYS coupled-field analysis, the total strain relevant to the process of electromigration is a sum of elastic strain

$\boldsymbol{\varepsilon}^{el}$ , thermal strain  $\boldsymbol{\varepsilon}^{th}$ , and diffusion expansion strain  $\boldsymbol{\varepsilon}^{di}$  as follows,

$$\boldsymbol{\varepsilon} = \boldsymbol{\varepsilon}^{el} + \boldsymbol{\varepsilon}^{th} + \boldsymbol{\varepsilon}^{di} \quad (4)$$

where the diffusion expansion strain is defined as follows:

$$\boldsymbol{\varepsilon}^{di} = \beta(\bar{C} - C_{ref})\mathbf{I} \quad (5)$$

where  $\beta$  is the coefficient of diffusion expansion and  $C_{ref}$  is the reference concentration.

To illustrate the ANSYS's capabilities for modeling the distributions and evolutions of vacancy concentration and stress, a 1-D model of electromigration in pure metal line was performed in this paper. As shown in the paper [27], the coefficient of diffusion strain is set as  $\beta = -0.05$  to obtain a "reasonable" hydrostatic stress value at steady state ( $\sim 350$  MPa), but this value of  $\beta$  is given without any reference and basis. Furthermore, by using the vacancy diffusivity  $D_v = 3 \times 10^{-16}$  m<sup>2</sup>/s, the predicted time to reach steady state is "comparable" with the experimental results. However, the vacancy diffusivity of Al is experimentally measured in the scale of  $10^{-9}$  m<sup>2</sup>/s.

In the following, we will first introduce the general couple model of electromigration we developed recently [25], and then we will use current ANSYS coupled-field modeling capability to correctly simulate electromigration behavior.

### III. IMPLEMENTATION OF GENERAL COUPLING MODEL

#### A. General Coupling Model of Electromigration

The details and full equations of the general coupling model are presented in the paper [25] (*J. Appl. Phys.* 125, 105101, 2019). Here, we highlight some key equations. In general coupling model, the transport equation of electromigration is written as follows:

$$\frac{\partial \theta}{\partial t} = \Omega \nabla \cdot \mathbf{J}_v \quad (6)$$

where  $\theta$  is the trace of total strain that is the sum of elastic strain  $\boldsymbol{\varepsilon}^{el}$ , thermal strain  $\boldsymbol{\varepsilon}^{th}$ , and electromigration strain  $\boldsymbol{\varepsilon}^{em}$ . If we neglect the thermal effects, the transport equation can be rewritten as follows,

$$\frac{\partial \boldsymbol{\varepsilon}_{kk}^{em}}{\partial t} + \frac{\partial \boldsymbol{\varepsilon}_{kk}^{el}}{\partial t} = \Omega \nabla \cdot \mathbf{J}_v \quad (7)$$

The formulation of electromigration induced strain in the general coupling model is written as the following equation, which can be linearized,

$$\begin{aligned} \boldsymbol{\varepsilon}^{em} &= -\frac{A}{3} \ln\left(\frac{C_v}{C_{v0}}\right)\mathbf{I} \\ &\approx -\frac{A}{3} \left(\frac{C_v}{C_{v0}} - 1\right)\mathbf{I} \end{aligned} \quad (8)$$

where  $A$  is the coefficient of electromigration strain and  $C_v/C_{v0}$  is the normalized vacancy concentration. Comparing Eq. (8) with (5), the linear form of electromigration strain is corresponding to the formulation of diffusion strain in ANSYS.

Applying Eq. (8) to Eq. (7), we can obtain the following expanded transport equation,

$$-\frac{A}{C_{v0}} \frac{\partial C_v}{\partial t} + \frac{\partial \boldsymbol{\varepsilon}_{kk}^{el}}{\partial t} = \Omega \nabla \cdot \mathbf{J}_v \quad (9)$$

To implement the general coupling theory in ANSYS, certain approximations are needed. Here, we assume the following relationship between volumetric elastic strain and electromigration strain,

$$\boldsymbol{\varepsilon}_{kk}^{el} = K \boldsymbol{\varepsilon}_{kk}^{em} \quad (10)$$

where the coefficient  $K$  may be determined through material properties, geometry features of conductor and mechanical boundary condition. For a 1-D metal line, if there is no any constraint on the metal line (stress-free configuration), the elastic deformation the metal line is zero. For the metal line embedded in a rigid passivation layer, the metal line is totally fixed. Thus,  $K$  can be approximately obtained as follows [25],

$$K = 0 \quad (\text{Stress-free condition}), \quad (11)$$

$$K = -\frac{2(1-2\nu)}{3(1-\nu)} \quad (\text{rigid passivation layer}), \quad (12)$$

where  $\nu$  is the Poisson's ratio of the conductor. Thus, the value of  $K$  is between "0" and " $-2(1-2\nu)/3(1-\nu)$ ".

Applying Eq. (10) to Eq. (9), the vacancy transport equation using general coupling model can be rewritten as the following equation,

$$\begin{aligned} \frac{\partial \bar{C}_v}{\partial t} &= -D_{eff,v} \nabla \cdot (-\nabla \bar{C}_v + \frac{Z^* e E \bar{C}_v}{kT}) \\ &\quad - \frac{\Omega}{kT} \bar{C}_v \nabla \cdot \boldsymbol{\sigma} + \frac{Q^*}{kT^2} \bar{C}_v \nabla T \end{aligned} \quad (13)$$

where:

$$D_{eff,v} = \frac{C_{v0}\Omega}{(1+K)A} D_v \quad (14)$$

Comparing Eq. (3) with Eq. (13), the governing equation using general coupling model is identical to the vacancy transport equation in ANSYS, except the vacancy diffusivity. Please note that the sink/source term is not shown in the governing equation (13), but the effect of sink/source term on the time scale of electromigration is taken into account via the effective vacancy diffusivity as shown in Eq. (14).

### B. Methods to implement general coupling model of electromigration in ANSYS

We can use the current ANSYS build-in coupled-field modeling theory to implement the general coupling model for electromigration in ANSYS, as summarized in Table I.

For the strain induced by atomic diffusion, as the electromigration strain in general coupling model is corresponding to the diffusion strain in ANSYS, thus the coefficient of diffusion expansion strain  $\beta$  is set based on the coefficient of electromigration strain ( $-A/3$ ) and  $C_{ref}$  is set as "1". For the governing equation of vacancy transport, the diffusivity  $D_v$  in ANSYS is replaced by the effective diffusivity  $D_{eff,v}$ .

TABLE I. METHODS TO IMPLEMENT GENERAL COUPLING MODEL IN ANSYS

Term	GCM (General Coupling Model)	ANSYS build-in coupling theory
Diffusion Strain	Eq. (8)	Eq. (5)
	By setting $\beta = -A/3$ and $C_{ref}=1$	
Transport Equation	Eq. (13)	Eq. (3)
	By setting $D_v = D_{eff,v}$	

## IV. CASE STUDY

### A. Benchmark problem

A 1-D totally confined metal line with perfectly blocking condition is studied as a benchmark problem, as shown in Fig.1. For the sake of simplicity, the Joule heating effect is ignored in this study, thus no temperature gradient for the entire model. Table II shows the material properties of metal line. Table III shows inputs parameters of migration model used in present study.

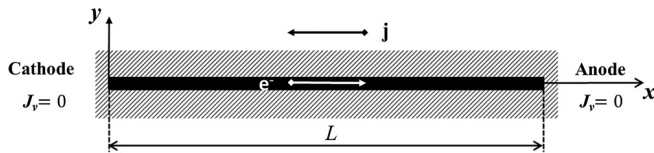


Figure 1. Benchmark problem for a metal line embedded in a rigid passivation layer.

Following initial and boundary conditions are implied:

- Initial condition:  $C_v(x) = C_{v0}$  and  $T = 475K$ .
- Diffusion boundary condition: the vacancy flux is blocked at both sides of metal line,  $J_v(0) = J_v(L) = 0$ .
- Mechanical boundary condition: metal line is embedded in a rigid passivation layer,  $u_y = u_z = 0$  and  $u_x(0) = u_x(L) = 0$ .

TABLE II. MATERIAL PROPERTIES

Length of the metal line ( $L$ )	50 $\mu\text{m}$
Young's modulus ( $E$ )	70 GPa
Poisson ratio ( $\nu$ )	0.3
Initial vacancy concentration ( $C_{v0}$ )	$6.0 \times 10^{21} \text{ m}^{-3}$
Vacancy diffusivity ( $D_v$ )	$3.0 \times 10^{-9} \text{ m}^2/\text{s}$
Atomic diffusivity ( $D_a$ )	$3.0 \times 10^{-16} \text{ m}^2/\text{s}$
Atomic volume ( $\Omega$ )	$1.66 \times 10^{-29} \text{ m}^3$
Electrical resistivity ( $\rho$ )	$4.88 \times 10^{-8} \text{ Ohm}\cdot\text{m}$
Current density ( $j$ )	$1.0 \times 10^{10} \text{ A}/\text{m}^2$
Elementary charge ( $e$ )	$1.6 \times 10^{-19} \text{ C}$
Charge number ( $Z^*$ )	3.5
Boltzmann constant ( $k_B$ )	$1.38 \times 10^{-23} \text{ J}/\text{K}$
Coefficient of electromigration strain ( $A$ )	0.0071
Ratio between $\epsilon^{el}$ and $\epsilon^{em}$ ( $K$ )	-0.38

TABLE III. INPUTS OF MIGRATION MODEL IN PRESENT STUDY.

Term	Inputs parameters
Coefficient of diffusivity	mp, dxx, $\frac{C_{v0}\Omega}{(1+K)A} D_v$
Coefficient of diffusion expansion	mp, betx, 1, $-A/3$
Reference concentration	mp, cref, 1, 1
Option of migration model	tb, migr, 1,,1
Parameter for stress-migration	tbdata, 2, $\Omega/k_B$
Parameter for electromigration	tbdata, 4, $Z^*/k_B$

### B. Results

The electromigration analysis is performed by using the field variable  $C_v(x)$  and the SOLID226 element with KEYOPT(1)=100101. To verify the FE results, the analytical solution of this 1-D problem obtained in paper [25] is used to compare with the FEA results.

Fig.2(a) plots the normalized vacancy concentration along the length of metal line, in which vacancies accumulate on the cathode side and decrease on the anode side. This indicates that atoms transport along the opposite direction of the current density. Fig. 2(b) shows the tensile stress on the cathode side due to the depletion of atoms, and the compressive stress on the anode side. At the steady state, the FEA results are in excellent agreement with the numerical results obtained from analytical solutions. Also,

the transient-state results of FEA are consistent with the results of analytical solutions, as shown in Fig. 3 (a) and (b).

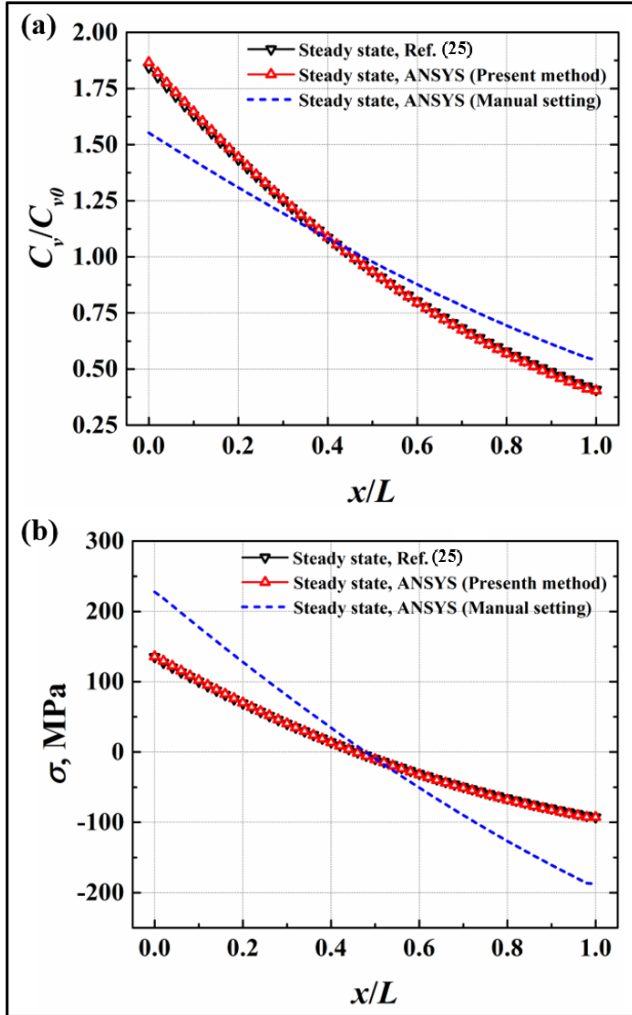


Figure 2. (a) Distribution of vacancy concentration along the length of conductor. (b) Distribution of hydrostatic stress along the length of conductor.

In addition, present results show obvious differences with the results obtained by using the benchmark setting given in ANSYS manual. At steady state, a higher vacancy concentration ( $1.85C_{v0}$  vs.  $1.56C_{v0}$ ) and lower hydrostatic stress (134 MPa vs. 225 MPa) are obtained. It is because that the APDL input file shown in ANSYS manual gives a fully confined mechanical condition to entire metal line, in which each point in metal line is totally fixed, thus the volumetric strain is zero everywhere. However, in the present finite element analysis, the mechanical boundary condition at  $x$ -direction is set as  $u_x(0)=u_x(L)=0$ , which means that the volumetric strain in local area can vary along the line and is not zero, but the integral over the entire length is zero. Thus, the mechanical boundary condition in ANSYS manual setting is over constraint compared to the present condition.

Furthermore, the predicted lifetime to reach steady state, by using the ANSYS manual setting, is about 500s that is

much shorter than the lifetime in the present study. It is because the diffusivity coefficient controls the time to reach the steady state: the greater the diffusivity coefficient, the faster the steady state is reached. In present implementation, as the effect of sink/source term on electromigration is considered by using the effective vacancy diffusivity  $D_{eff,v}$ , thus the time to reach a steady-state concentration takes few hours. However, for the vacancy diffusivity coefficient  $D_v \approx 10^5 D_{eff,v}$  used in Eq. (3), the steady-state can be achieved in a few hundred seconds, and this lifetime actually is too short—several orders shorter than the experimental results.

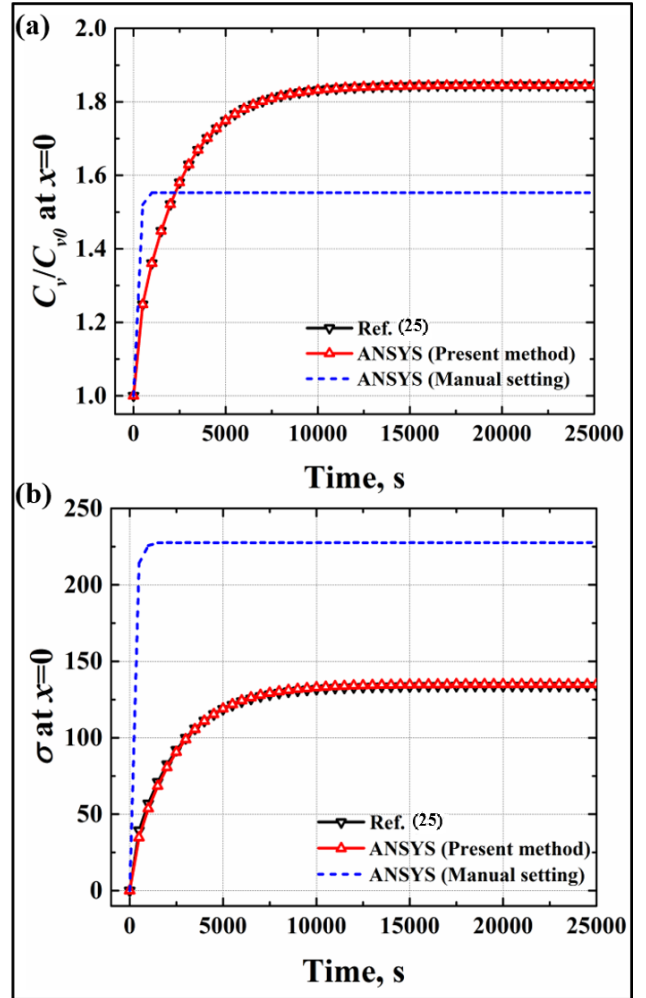


Figure 3. (a) Vacancy concentration buildup over time at  $x=0$ . (b) Hydrostatic stress buildup over time at  $x=0$ .

Fig. 4 illustrates the buildup of normalized vacancy concentration over time with different  $K$ . For the coefficient  $K=0$ , its steady state is reached at  $\sim 5000$ s that is faster than the model with  $K=-0.38$  ( $\sim 8000$ s). But both models show that vacancy concentrations evolve on the same time scale, and the same steady-state results are obtained. Thus, the coefficient  $K$  only affects the time to reach steady state of electromigration, no effect on the steady-state solution.

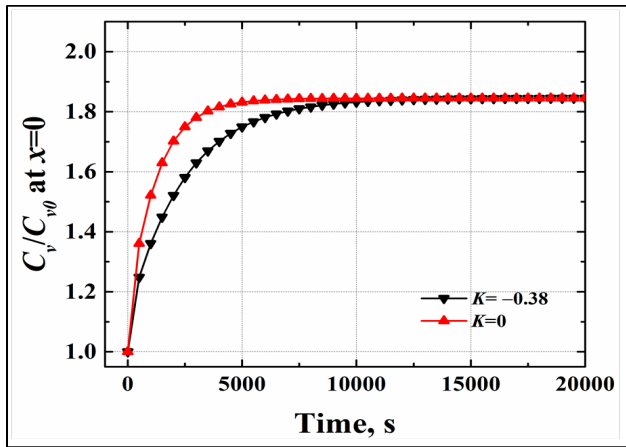


Figure 4. Evolution of normalized vacancy concentration over time at  $x=0$  with two different values of  $K$ .

### CONCLUSION

In this paper, a newly developed general coupling model for electromigration is implemented in ANSYS by using the ANSYS build-in coupled-field theory. Several incorrect settings in ANSYS manuals are identified and corrected. The details of the implementation of the general coupling model in ANSYS are presented. As a validation, the obtained 1-D FE solutions are in excellent agreement with the analytical solutions. Although the sink/source term is not used, the effect of this term is considered through the adjustment of the diffusivity with some approximations.

### ACKNOWLEDGMENT

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