Two-dimensional Analysis of Triple Coupled Physics of Structural Mechanics, Diffusion and Heat Transfer in a Gas Pipe

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Abstract: In this study, a 2-D model has been built using COMSOL Multiphysics® to analyze a triple coupled physics problem involving simultaneous gas diffusion, heat transfer, and structural mechanics in a pipe due to the flow of high-pressure carbon dioxide. The problem geometry and boundary conditions were based on the analysis by Rambert *et al.* who have published the most advanced modeling work in the open literature. Comparison of results with the Rambert group's work showed excellent agreement. It will be demonstrated that COMSOL Multiphysics® software offers a more efficient and user friendly capability for solving complex multiphysics problems.

Keywords: Multiphysics modeling, structural mechanics, mass diffusion, heat transfer, COMSOL Multiphysics.

1. Introduction

In the past thirty years, polymeric materials have increasingly been used to manufacture components and structures for various industrial applications such as electronics and mobile telecommunication industries, oil and gas industry, aerospace industry, and automobile industry. These materials are, therefore, subjected to a range of in-service environmental conditions that can adversely affect their properties and durability. Generally, the mechanisms responsible for the degradation of material properties are complex and involve more than one physical phenomenon. The prediction of material behavior, therefore, needs consideration of multiple physics simultaneously. The problem becomes more challenging when these physics are coupled, i.e., the prediction of one physical mechanism depends on knowing the effect of the other and vice versa. A very common example of coupled physics is the coupling between heat transfer and structural mechanics, where the stresses induced in a structure caused by thermal changes can only be obtained by conducting an analysis of the temperature distribution in the structure.

Similarly, diffusion of moisture and gases into polymeric materials is usually accompanied by heat transfer and mechanical deformation, and these three physical mechanisms have interacting effects on material behavior. To model the coupled behavior, researchers have applied different approaches, which were mostly based on the capabilities of the software packages. Some have used existing modules of finite element modeling packages for thermo-mechanical analysis to model the coupled behavior of mass diffusion and structural mechanics using the similarity between heat and mass transfer. For instance, Wong *et al.* [1] used this technique to characterize the hygroscopic swelling of polymeric materials during solder reflow in electronic packages. Moisture induced failure of adhesive flip chip was investigated using the same method by Teh *et al.* [2]. In their work, finite element analysis was used to study the effect of the coefficient of moisture expansion mismatch on hygroscopic swelling stress induced in the package.

Similarly, some authors have used an equivalent coefficient of thermal expansion, which includes both thermal and hygroscopic swelling strain. Lahoti *et al.* [3] used this technique and treated the hygroscopic swelling strain as an additional "thermal strain". A 3D-finite element analysis was applied to study the effect of temperature and moisture on the reliability of flip chip ball grid array packages. Holalkere *et al.* [4] in their study of plastic package delamination used finite element stress analysis together with fracture mechanics to evaluate moisture sensitivity of plastic encapsulated microcircuits. In the procedure they employed, the molding compound swelling was also treated as an equivalent thermal expansion.

Sequentially coupled analyses is another technique for modeling the coupled physics of mass diffusion and structural mechanics. In this technique a transient mass diffusion analysis is done first and the results from this analysis are considered as loads in subsequent structural analysis. Zhou [5] adopted this method in a study on accurate determination of the coefficient of hygroscopic swelling and simulated the hygroscopic swelling characterization process of polymeric materials.

A so-called *fully coupled analyses* is a powerful method in modeling coupled physics, which has been employed by some authors [6-10]. This method involves simultaneous solving of coupled governing equations and therefore, considers the interacting couplings between different physical mechanisms at the same time. Rambert *et al.* [6] presented a mechanical-diffusion-thermal model using this approach. The model was developed based on the framework of classical thermodynamics and a set of coupled constitutive equations was derived for linear elastic behavior. Rambert *et al.* [6] employed finite element analysis of ABAQUS® for numerical implementation of the direct coupling in the governing equations and developed a user-defined element (UEL) for this purpose. The technique they have applied considers the coupling between the three physics involved in the problem; however, the software package they employed requires developing a new type of element for analysis using programming packages such as Intel® FORTRAN, which renders the modeling more complicated and less flexible. Nevertheless, as far as the authors know, Rambert's group has published the most advanced work in this area.

Multiphysics modeling including heat and mass transfer as well as elastic solid mechanics using COMSOL Multiphysics® was recently applied by Niamnuy *et al.* [11] to model heat conduction, mass diffusion, and elastic solid mechanics of shrinkable and irregular-shape biomaterials, such as shrimp during drying, by coupling *chemical engineering* and *structural mechanics* modules. They found good agreement between their modeling results and experimental results.

The purpose of this study is to investigate the capability of COMSOL Multiphysics® for analyzing the triple coupled physics of structural mechanics, diffusion, and heat transfer in a gas pipe using the constitutive equations developed by Rambert *et al.* [6]. In the following sections, the background on diffusion and the governing equations of the three coupled physics are described. A framework on how COMSOL Multiphysics® was used to build up the model for conducting a parametric analysis of the problem is then provided, followed by comparison with the results of Rambert *et al.*, which have already been experimentally verified by other researchers in the field [10].

2. Theory and Governing Equations

The first and the most well-known theory for diffusion was presented by Fick in 1855, based on an analogy between diffusion and heat flow, as the following [12]:

$$\boldsymbol{J} = -\boldsymbol{D}\frac{\boldsymbol{dC}}{\boldsymbol{dx}} \qquad (1)$$

where J and C are the flux and concentration of the diffusion species, respectively; and D is known as *diffusion coefficient*. The above equation expresses a steady state diffusion in a one-dimensional system (direction x) and is referred to as Fick's first law of diffusion.

Fick's second law of diffusion introduces a relation for non-steady state diffusion, as follows [12]:

$$\frac{\partial \boldsymbol{C}}{\partial \boldsymbol{t}} = \frac{\partial}{\partial \boldsymbol{x}}\left(\boldsymbol{D}\frac{\partial \boldsymbol{C}}{\partial \boldsymbol{x}}\right) \qquad (2)$$

Fick's first and second laws of diffusion express the type of diffusion which is driven by concentration gradient, $\partial C/\partial x$. However, when the diffusant enters a polymer, the polymer may be deformed and stress builds up in the material. This stress causes the diffusant molecules to move from high stress regions to low stress regions [13]. This effect, which is also referred to as *pressure effect,* shows how the two physical mechanisms interact. Similarly, temperature gradient can also cause mass diffusion. This effect, known as *Soret effect*, shows the coupling between mass diffusion and heat transfer.

Rambert *et al.* [6-9] in their modeling of coupling between the three physics of heat transfer, gas diffusion, and structural mechanics considered all the direct couplings among the physics in the classical framework of thermodynamics of irreversible processes. They considered the simplest model for the mixture of gas and polymer and derived the constitutive equations by developing the balance laws of mass, mechanical, and thermodynamics for the mixture. The equation derivations can be found in references [6-8]. The governing equations are as follows [7]:

$$\boldsymbol{S} = \boldsymbol{S_o} + \lambda(tr\boldsymbol{E^e})\boldsymbol{I} + 2\mu\boldsymbol{E^e} - (3\lambda + 2\mu)[\alpha^T \Delta T + \alpha^D \Delta Y_g]\boldsymbol{I} \tag{3}$$

$$\begin{aligned}\rho_o s_g \dot{Y}_g &= \rho_o D s_g \,Div[\nabla Y_g] + [K_{T\mu} - C_{TY} K_\mu]\, Div[\nabla T] \\ &\quad - K_\mu \alpha^D \frac{(3\lambda + 2\mu)}{\rho_o} Div[\nabla(trE^e)]\end{aligned} \tag{4}$$

$$\begin{aligned}\rho_o C_T \dot{T} &= [\lambda_T + C_{TY} T (C_{TY} K_\mu - 2K_{T\mu})]\, Div[\nabla T] \\ &+ q - (3\lambda + 2\mu)\alpha^T T tr\dot{E}^e \\ &+ (K_{T\mu} - C_{TY} K_\mu)\frac{\rho_o D s_g}{K_\mu} Div[\nabla Y_g] \\ &- (K_{T\mu} - C_{TY} K_\mu) T \alpha^D \frac{(3\lambda + 2\mu)}{\rho_o} Div[\nabla(trE^e)] \\ &+ (C_{TY} K_\mu - 2K_{T\mu}) C_{TY} [\nabla T]^2 + \frac{(\rho_o D s_g)^2}{K_\mu}[\nabla Y_g]^2 \\ &+ K_\mu \left[\alpha^D \frac{(3\lambda + 2\mu)}{\rho_o}\right]^2 [\nabla(trE^e)]^2 \\ &+ 2(K_{T\mu} - C_{TY} K_\mu)\frac{\rho_o D s_g}{K_\mu} \nabla T . \nabla Y_g \\ &- 2(3\lambda + 2\mu) D s_g \alpha^D \nabla Y_g . \nabla(trE^e) \\ &- 2(K_{T\mu} - C_{TY} K_\mu)\alpha^D \frac{(3\lambda + 2\mu)}{\rho_o} \nabla T . \nabla(trE^e)\end{aligned} \tag{5}$$

The definitions of the notations used in the equations above are presented in Table 1.

Table 1: Definition of notations used in equations (3)-(5)

Notation	Definition
α^D	Coefficient of hygroscopic expansion
α^T	Coefficient of thermal expansion
λ, μ	Lamé constants
λ_T	Thermal conductivity
ρ_o	Average mixture density
C_T	Specific heat
C_{TY}	Coefficient representing the effect of temperature (concentration) variation on the chemical potential (entropy)
D	Diffusivity
E^e	Elastic strain tensor
K_μ	Coefficient linked to the chemical potential gradient effect on the gas mass flux
$K_{T\mu}$	Coefficient corresponding to the temperature (chemical potential) gradient effect on the mass (entropy) flux
q	Volume density of heat generated by an external source
s_g	Solubility coefficient of gas in polymer
S	Cauchy stress tensor
S_o	Initial Cauchy stress tensor
T	Temperature
Y_g	Mass fraction of gas

Equations (3)-(5) are the constitutive equations of structural mechanics, mass diffusion, and heat transfer, respectively, in which five coupling coefficients (α^T,α^D, K_μ, $K_{T\mu}$, C_{TY}) relate the equations to one another.

3. Application of COMSOL Multiphysics

In order to model the three coupled physics in COMSOL Multiphysics 3.5a, a known example problem has been investigated. A two-dimensional model was developed for a gas pipe, Figure 1, to facilitate parametric analysis of coupling conditions. The pipe geometry, which is identical to that used by Rambert *et al.* [6-8], has an internal diameter of 5 mm and a thickness of 1 mm. Because of the symmetry of the pipe only a quarter of it has been modeled.

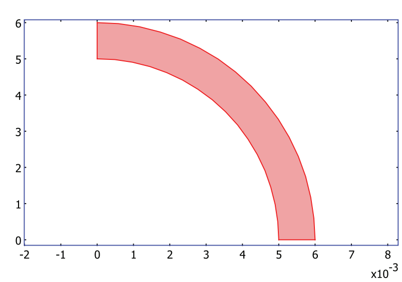

Figure 1. The geometry of the quarter of the pipe modeled with COMSOL Multiphysics.

In this analysis, the pipe is made of polyvinylidene fluoride (PVDF) with material characteristics presented in Table 2. Following Rambert *et al.* [6], the pipe was assumed to behave in a linear elastic manner.

Table 2: Material characteristics of a PVDF sample and CO_2 at 21 °C [7]

Parameter	Value	Parameter	Value
ρ_o (kg/m^3)	1745	α^T (K^{-1})	10^{-5}
λ (MPa)	2000	s_g (Pa^{-1})	5.539×10^{-9}
μ (MPa)	631	d (m^2/s)	9.8×10^{-12}
C_T (J/kg.K)	1045	α^D (∅)	2.2×10^{-13}
λ_T (W/m.K)	0.26		

The pipe is used for transporting carbon dioxide (CO_2) and therefore, is under internal pressure, temperature, and gas concentration variations. The boundary conditions and initial conditions as well as loading diagrams are shown in Figures 2 and 3, respectively.

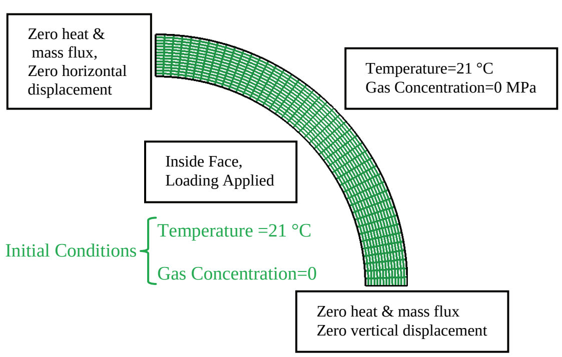

Figure 2. Meshed pipe model with boundary conditions and initial conditions (adopted from reference [7]).

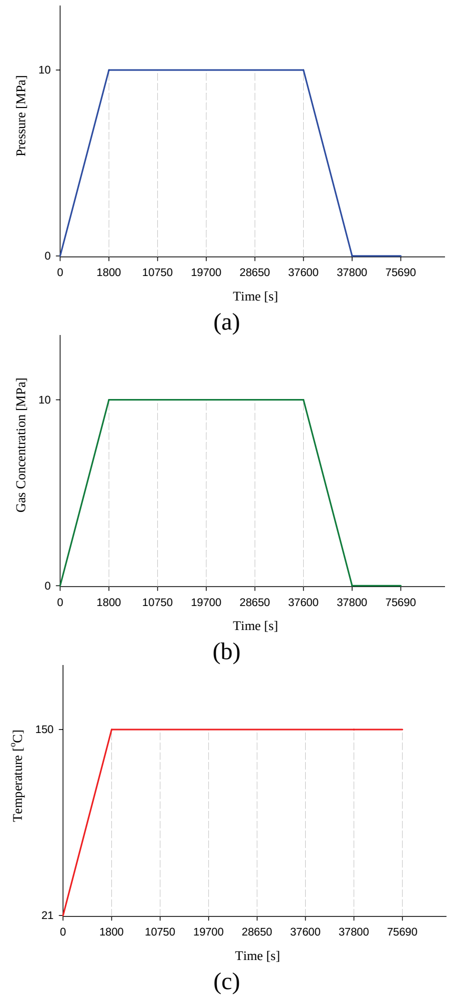

Figure 3. Applied loading diagrams on the inside face of the pipe, (a) Pressure, (b) Gas Concentration, (c) Temperature (adopted from reference [6]).

In order to model the three coupled physics with the governing equations of (3) to (5), a *Multiphysics* model was formed in the *Model Navigator*. Since the analysis is two dimensional and the pipe is subjected to plane strain condition, the *transient analysis* of *plane strain mode* is selected from the *Structural Mechanics Module*. This application mode, however, only models the mechanical stress of equation (3) (the first three terms on the right hand side). Therefore, to model the stresses caused by temperature and gas concentration changes $((3\lambda+2\mu)(\alpha^T\Delta T+\alpha^D\Delta Y_g))$, the *Equation System* of *Subdomain Settings* was modified.

Since equations (4) and (5) are in the form of partial differential equations (PDE), the most suitable application mode for modeling them is the *PDE Mode*. Equation (4), which describes the behavior of gas diffusion, is a linear PDE and therefore can be modeled using a PDE in the *coefficient form*. Equations (5), however, is a nonlinear PDE and is therefore best modeled with a PDE in the *general form*. The *coefficient* and *general* forms of the PDEs have the following forms [14]:

$$\boldsymbol{e_a}\frac{\partial^2 \boldsymbol{Y_g}}{\partial \boldsymbol{t}^2}+\boldsymbol{d_a}\frac{\partial \boldsymbol{Y_g}}{\partial \boldsymbol{t}}+\nabla.\left(-\boldsymbol{c}\nabla \boldsymbol{Y_g}-\alpha \boldsymbol{Y_g}+\gamma\right)+\boldsymbol{a}\boldsymbol{Y_g}+\beta.\nabla \boldsymbol{Y_g}=\boldsymbol{f} \qquad (6)$$

$$\boldsymbol{e_a}\frac{\partial^2 \boldsymbol{T}}{\partial \boldsymbol{t}^2}+\boldsymbol{d_a}\frac{\partial \boldsymbol{T}}{\partial \boldsymbol{t}}+\nabla.\Gamma=\boldsymbol{F} \qquad (7)$$

The coefficients of the equations above were formulated such that the equations led to constitutive equations for mass diffusion and heat transfer; i.e., equations (4) and (5). Therefore the parametric terms, such as $\partial \boldsymbol{T}/\partial \boldsymbol{x}$ (=*d(T,x)*) were defined as *Global* and *Scalar Expressions* and were used as the coefficients of equations (6) and (7).

In order to conduct a parametric study, all the constants including the five coupling coefficients (α^T,α^D, K_μ, $K_{T\mu}$, C_{TY}) were defined as *Constants*. This made it possible to readily change the value of a parameter in the *Constants* window for a new analysis.

A *Time dependant* solver was selected for solving the problem and the *UMFPACK Direct Solver* was selected as the *Linear System Solver*.

The uncoupled models were first developed and the results were compared with the models developed using existing models of COMSOL Multiphysics® as well as those obtained from Abaqus® models. The good agreement between the results of these models showed that the PDEs have been correctly defined. Next, the coupled models were solved by successively introducing the five coupling coefficients (α^T,α^D, K_μ, $K_{T\mu}$, C_{TY}) to the model. The results were then compared with those obtained from the parametric study reported by Rambert *et al.* [6].

4. Results and Discussion

The effects of different values of the coupling coefficients on displacement, gas concentration, and temperature were investigated and the results were compared with the results reported by Rambert *et al.* [6]. Figure 4 shows the effect of the coupling coefficient C_{TY} on gas concentration at radius of 5.25 mm of the pipe at different times. For comparison, a diagram extracted from the work of Rambert *et al.* [6] is presented in Figure 5.

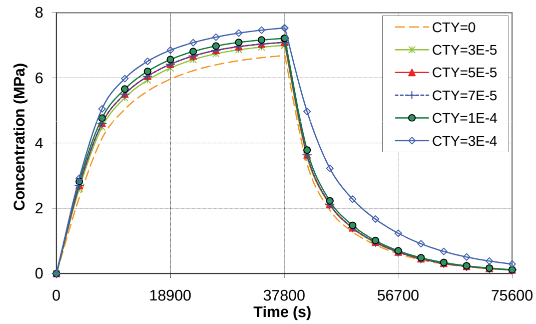

Figure 4. The effect of different values of C_{TY} on concentration at the radius of 5.25 mm as modeled by COMSOL Multiphysics.

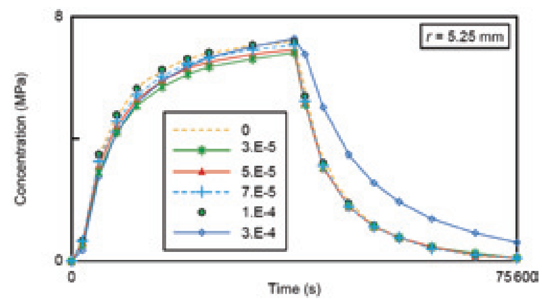

Figure 5. Effects of $K_{T\mu}$ and C_{TY} on the diffusion problem for $K_\mu = 10^4$ kg.s/m^3, $K_{T\mu} = 1$ kg/(m.s.K) and various C_{TY} [6].

Comparison between Figures 4 and 5 shows that the developed model in COMSOL Multiphysics® is capable of modeling the triple coupled physics for the most complicated case; i.e., the case where all the coupling coefficients are nonzero.

Similarly, the effect of different values of C_{TY} on temperature and radial displacement at radius 5.25 mm of the pipe at different times was investigated. The obtained results and the corresponding figures from the work of Rambert *et al.* [6] are depicted in Figures 6 to 9.

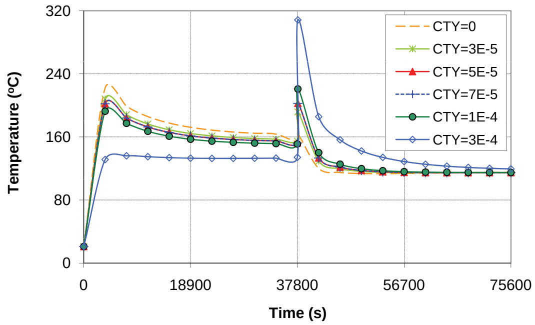

Figure 6. The effect of different values of C_{TY} on temperature at the radius of 5.25 mm as modeled by COMSOL Multiphysics.

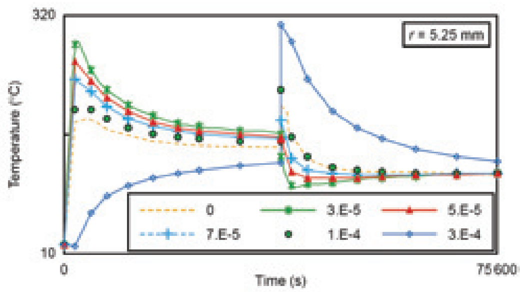

Figure 7. Effects of $K_{T\mu}$ and C_{TY} on the thermal problem for $K_\mu = 10^4$ kg.s/m^3, $K_{T\mu} = 1$ kg/(m.s.K) and various C_{TY} [6].

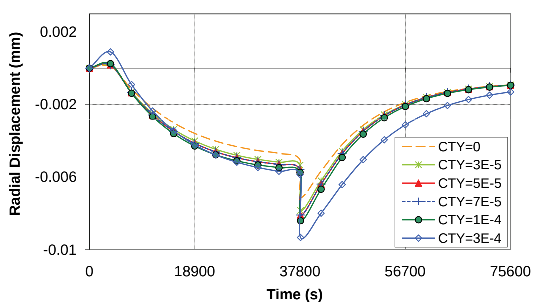

Figure 8. The effect of different values of C_{TY} on radial displacement at the radius of 5.25 mm as modeled by COMSOL Multiphysics.

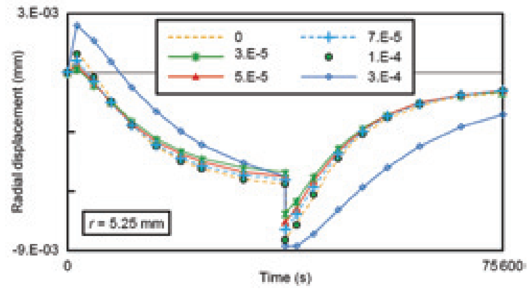

Figure 9. Effects of $K_{T\mu}$ and C_{TY} on the mechanical problem for $K_\mu = 10^4$ kg.s/m^3, $K_{T\mu} = 1$ kg/(m.s.K) and various C_{TY} [6].

As seen in Figures 6-9, the trend of the curves are very similar between those modeled by COMSOL Multiphysics® and those presented by Rambert *et al.* [6]. The values of the curves are also very similar; however, there are minor differences in the values that are inherent in finite element analysis. The differences can be due to different mesh sizes, different time steps, and different solution methods.

5. Conclusions

Finite element analysis of a relatively complicated tripled coupled multiphysics problem for a polymeric material has been conducted using COMSOL Multiphysics® software package. The developed two-dimensional analysis of coupled physics of structural mechanics, gas diffusion, and heat transfer in a gas pipe was readily implemented. COMSOL Multiphysics® allowed a complete parametric study of the problem and generated results which agreed very well with the most advanced work in the literature, namely by the Rambert group. This work has demonstrated that the software package has significant potential for analyzing even more complicated mechanisms such as viscoelastic analysis, which is known to be computationally intensive and time consuming.

6. References

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