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МНОГОМАСШТАБНОЕ МОДЕЛИРОВАНИЕ ПОНИЖЕННОГО ПОРЯДКА ДЛЯ ИССЛЕДОВАНИЯ ДЕГРАДАЦИИ КОМПОЗИЦИОННЫХ МАТЕРИАЛОВ ПОД ДЕЙСТВИЕМ ВЛАГИ

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Аннотация

Имеется множество факторов, влияющих на деградацию композиционных материалов под действием окружающей среды. В настоящей работе изучается два источника деградации. Во-первых, мы исследуем накопление повреждений в материале, состоящем из углеродных волокон и эпоксидной смолы, при циклическом нагружении. Во-вторых, развит многомасштабный и мультифизический подход к исследованию деградации материала, состоящего из стекловолокна и нейлона, вследствие накопления влаги. Мультифизический и многомасштабный подход учитывает совместное протекание реакционно-диффузионных и механических процессов на нескольких масштабных уровнях.

Ключевые слова: Композиционные материалы, многомасштабный многофизический подход, деградация композиционных материалов.

Библиография: 24 название.

REDUCED ORDER MULTISCALE ANALYSIS OF MOISTURE DEGRADATION IN COMPOSITE MATERIALS

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Abstract

There are variety of factors affecting degradation of composite materials due to environmental effects. In the present manuscript, two sources of degradation are studied. We first consider an accumulation of damage in carbon-fiber/epoxy-resin material system subjected to cyclic load. A

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multiscale-multiphysics approach is developed for degradation of glass-fiber/Nylon material system due to moisture accumulation. A multiphysics-multiscale approach couples diffusion-reaction-mechanical process at multiple spatial scales.

Keywords: Composite materials, multi-scale multi-physical approach, degradation of composite materials.

Bibliography: 24 titles.

1. Introduction

Composites are widely used in aircraft, automotive and other industries due to their light weight, high strength and stiffness. Behavior of composite materials subjected to various environmental effects is not fully understood due to variety of factors, chief among them is understanding of the complex interplay between multiple spatial and temporal scales and interacting multiple physical processes. Herein, we focus on accumulation of moisture in glass-fiber/Nylon material system.

Considerable research efforts have been devoted towards developing predictive multiphysics simulation capabilities. For instance, Gerad et al. [1, 2] studied the coupling between chemical leaching in underground cementitious structures in the presence of water. Ulm et al. [3] pioneered a homogenization-based chemo-mechanical approach aimed at understanding the effect of chemical leaching on the structural integrity of concrete structures. Terada and Kurumatani [4] developed a two-scale diffusion-deformation model to analyze microcrack propagation and aging in quasi brittle solids in the presence of moisture. Yu and Fish [5] developed a space-time homogenization approach to resolve complex deformation processes in thermo-viscoelastic composites. Kuznetsov and Fish [6] devised an efficient coupling scheme between electrical and mechanical field in heterogeneous solids. In recent paper Klepach and Zohdi developed strongly-coupled, deformation-dependent diffusion model in composite media at finite strains [7]. This model based on computational multiphysics framework developed in [8, 9, 10]. Bailakanavar et al developed reduced order multiscale-multiphysics approach for chopped fiber composites [11]. An excellent treatise of coupled chemo-thermo-mechanical ageing processes of elastomers based thermodynamically coupled material model has been given by Johlitz and Lion. This work is based multiphase continuum theory [15–19] that finds its roots in earlier work of Truesdell [20].

Molecular processes occurring during penetration of fluid into a polymeric material systems are not well understood primarily due to lack of experimental data at that scale. There is no experimental data on mobility of polymer chains, their polarization, and configuration of free spaces occupied by the penetrant. Obviously, one can consider idealized scenarios with respect to molecular structure, and consequently postulate Gibbs free energy of mixtures, but without experimental backing for the material system of choice, such an approach will have limited practical use. Our goals are less ambitions in this regard. We will not postulate energy or entropy equations and will not attempt to derive a thermodynamically consistent framework for processes that presently are not well understood. The primary objectives are follows: (i) postulate physically motivated constitutive equations of the mechano-diffusion model at a microscale, i.e. at a level of microconstituents, i.e. fiber-matrix scale; (ii) upscale the coupled physics micromechanical model using classical mathematical homogenization theory; (iii) focus on model reduction of the two physical processes that would permit effective consideration of component scale (macro problems) having complex microstructure; (iv) identify model parameters appearing in the micromechanical model against uniform field macroscopic experiments, and (v) validate the model against more complex experiments (4-point bending problem).

We study degradation of glass-fiber/Nylon due to moisture accumulation. We consider coupling of three physical fields: diffusion and reaction of water with Nylon, and subsequent degradation of mechanical properties. The problem is a two-way coupled. On the one hand, water, which is absorbed by Nylon affects mechanical behavior. On the other hand, the mechanical damage accelerates diffusion of water. A first-order computational homogenization (FOCH) is employed for both diffusion-reaction and mechanical problems. Simulation results are compared to experimental measurements conducted at General Motors [21].

2. Diffusion-reaction process for glass-fiber-Nylon with moisture

2.1. Constitutive model of resin

Herein, we study environmental degradation of glass-fiber/Nylon material system caused by moisture accumulation, where water is absorbed by Nylon and, consequently, its strength decreases [22]. Water diffusion is enhanced by formation of microcracks. Thus, the process is a two-way coupled multiscale-multiphysics problem. The unit cell consists of random chopped fibers embedded in an epoxy resin as shown in Figure 1.

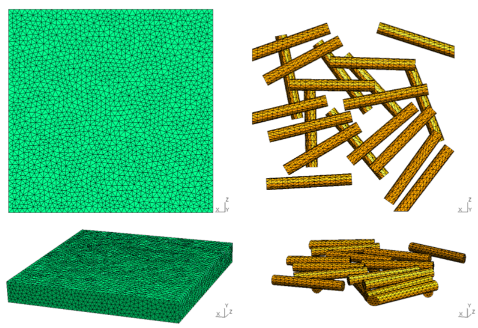

Рис. 1: Microstructure of random chopped glass fibers (right) embedded in the epoxy resin (left)

The process of absorption of Nylon and water molecules consists of two stages depicted in Figure 2. First, the reaction process, where one Nylon molecule absorbs three water molecules. Second, the diffusion process, where water molecule diffuses from high mass concentration to low mass concentration based on the Fick's law. The governing equations for the reaction-diffusion problem are given by

$$\begin{aligned} \dot{c}_w &= \nabla \cdot (\mathbf{D} \cdot \nabla c_w) + r_w\left(c_N, c_w\right) \\ \dot{c}_N &= r_N\left(c_N, c_w\right) \end{aligned} \tag{1}$$

where c_w and c_N denote the mass concentration of water and Nylon, respectively; $\mathbf{D}$ is the nonlinear diffusivity tensor. The reaction terms r_w and r_N are given by

$$\begin{aligned} r_w\left(c_N, c_w\right) &= -k \cdot c_N \cdot \left(c_w\right)^{3/2} \\ r_N\left(c_N, c_w\right) &= -k \cdot c_N \cdot \left(c_w\right)^{3/2} \end{aligned} \tag{2}$$

where k is a reaction coefficient.

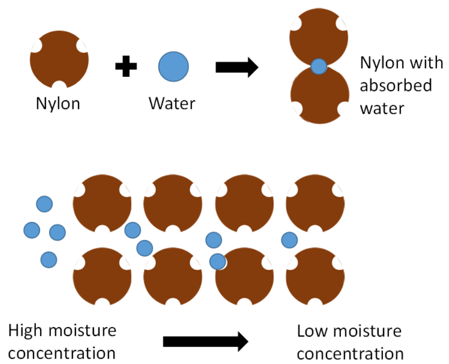

Рис. 2: Reaction (top) and diffusion (bottom) process of Nylon-water system

2.2. Model Reduction

To reduce the computational cost associated with multiple nonlinear unit cell solutions, the model reduction scheme process [22, 23] is employed. The model reduction technique is based on the construction of residual-free scalar (moisture diffusion) and vector (deformation) fields. The fine-scale perturbation of the displacement field $u_i^{(1)}$ is constructed to satisfy the unit cell equilibrium equations for arbitrary coarse-scale strains and eigenfields [23]

$$\begin{aligned} u_i^{(1)}\left(x,y,t\right) = H_i^{kl}(y)\varepsilon^c_{kl}(x,t) + \int_\Theta \tilde{h}_i^{kl}(y,\tilde{y})\mu^f_{kl}(x,\tilde{y},t)d\tilde{\Theta} + \\ + \int_S \breve{h}_i^{\breve{n}}(y,\breve{y})\delta^f_{\breve{n}}(x,\breve{y},t)d\breve{S} \end{aligned} \tag{3}$$

where H_i^{kl}, $\tilde{h}_i^{kl}$, and $\breve{h}_i^{\breve{n}}$ are the influence functions for the coarse-scale strains ε_{kl}^c, fine-scale eigenstrains μ_{kl}^f, and fine-scale eigenseparations $\delta_{\breve{n}}^f$, respectively.

Likewise, the fine-scale perturbation of the moisture concentration $c^{(1)}$ is constructed to satisfy the fine-scale diffusion equations for arbitrary coarse-scale concentration gradients $c_{,i}^c$ and fine-scale eigenconcentration gradient η_i^f as follows

$$c^{(1)}(x,\tilde{y},t) = H^i(y)c_{,i}^c(x,t) + \int\limits_{\Theta} h^i(y,\tilde{y})\eta_i^f(x,\tilde{y},t)d\tilde{\Theta} \tag{4}$$

where $H^i(y)$ and $h^i(y,\tilde{y})$ are the influence functions for the coarse-scale concentration gradient the eigenconcentration gradient, respectively. Inserting (3) and (4) into constitutive eqution yields

$$\left(L_{ijkl}(y)\begin{pmatrix}\left(I_{klmn} + H_{(k,y_l)}^{mn}\right)\varepsilon_{mn}^c(x,t) + \left(\int_{\Theta} \tilde{h}_{(k,y_l)}^{mn}(y,\tilde{y})\ \mu_{mn}^f(x,\tilde{y},t)d\tilde{\Theta} - \mu_{kl}^f(x,y,t)\right) \\ + \int_S \breve{h}_{(k,y_l)}^{\breve{n}}(y,\breve{y})\ \delta_{\breve{n}}^f(x,\breve{y})d\breve{S}\end{pmatrix}\right)_{,y_j} = 0 \tag{5}$$

$$\left(-D_{ij}'(y)\left(\left(I_{jk} + H_{,y_j}^k(y)\right)c_{,k}^c(x,t) + \left(\int\limits_{\Theta} h_{,y_j}^k(y,\tilde{y})\eta_k^f(x,\tilde{y},t)d\Theta - \eta_j^f(x,y,t)\right)\right)\right)_{,y_j} = 0 \tag{6}$$

The eigenstrains, eigenseparations and eigenconcentration gradients are discretized in terms of phase eigenstrains $\mu_{kl}^{(\alpha)}$, phase eigenseparations $\delta_{\hat{n}}^{(\alpha)}$ and phase eigenconcentration gradients $\eta_k^{(\alpha)}$ over the phase domain $\Theta^{(\alpha)}$ as follows

$$\begin{aligned} \mu_{ij}^f(x,y,t) &= \sum_{\alpha=1}^{n} \tilde{N}^{(\alpha)}(y)\mu_{ij}^{(\alpha)}(x,t) \\ \delta_{\breve{n}}^f(x,y,t) &= \sum_{\xi=1}^{m} \breve{N}^{(\xi)}(y)\delta_{\hat{n}}^{(\xi)}(x,t) \end{aligned} \tag{7}$$

$$\eta_k^f(x,y,t) = \sum_{\alpha=1}^{n} \tilde{N}^{(\alpha)}(y)\eta_i^{(\alpha)}(x,t). \tag{8}$$

The shape functions $\tilde{N}^{(\alpha)}(y)$ for the eigenstrain and eigenconcentration gradient are chosen to be $C^{-1}(\Theta)$ functions since the eigenfields can be discontinuous between the phases. The eigenseparation shape functions are chosen to be $C^0(S)$ functions since cracks (displacement jumps) should be continuous across the interfaces. The eigenstrain and eigenseparation shape functions are chosen as

$$\tilde{N}^{(\alpha)}(y) = \begin{cases} 1 & y \in \Theta^{(\alpha)} \\ 0 & y \in \Theta^{(\alpha)} \end{cases}, \qquad \breve{N}^{(\xi)}(y) = \begin{cases} \sum\limits_{A \in S^{(\xi)}} N_A^f(y) & y \in S^{(\xi)} \\ 0 & y \notin S^{(\xi)} \end{cases} \tag{9}$$

For more details we refer to [11, 24, 23].

2.3. Model validation

For validation, we study mechanical behavior of the glass-fiber/epoxy-resin material system subjected to moisture. The sample is exposed to moisture for 350 hours and then tested in a uniaxial tension. We will refer to such a sample condition as the moisture conditioned (MC) state. A dry-as-molded (DAM) sample state will be also tested for comparison.

The simulation of moisture conditioned (MC) samples will be divided into two steps: (i) simulation of diffusion-reaction process and (ii) simulation of a uniaxial tension till failure. A first-order computational homogenization (FOCH) approach is adopted for both diffusion-reaction and mechanical problems. Due to symmetry, the macroscopic model consists of one quarter of the sample as shown in Figure 3.

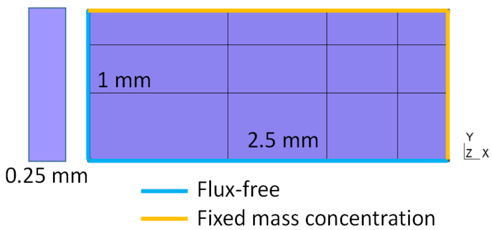

Рис. 3: Macroscopic model for the diffusion-reaction problem

Figure 4 compares the weight gain (%) as obtained by the simulation and physical experiments. It is evident that simulations predict correct amount of water absorption throughout the entire time history.

Next, we study mechanical behavior of DAM and MC samples in uniaxial tension up to failure. The comparison of simulated and experimental strain-stress curves is depicted in Figure 5 for the two states. The numerical model predicts correct mechanical response as well as the onset of failure. It can be seen that the peak stress (or strength) in DAM samples is higher than in MC samples. In contrast, the failure strain in DAM samples is lower than in the MC samples. Thus, the MC samples are more ductile than those of DAM.

A similar conclusion can be drawn by observing microscopic damage pattern depicted in Figure 6. The damage pattern exhibits brittle crack in DAM samples,

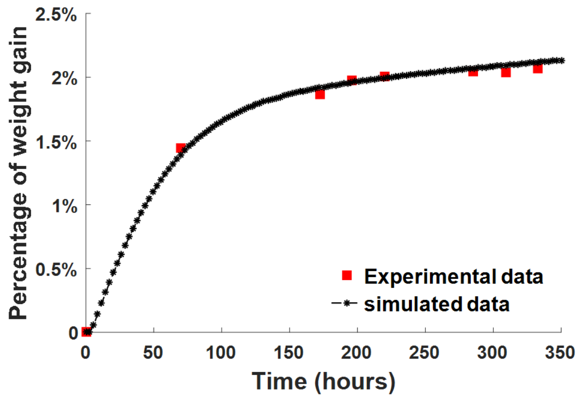

Рис. 4: Comparison of weight gain (%): experiments vs simulation

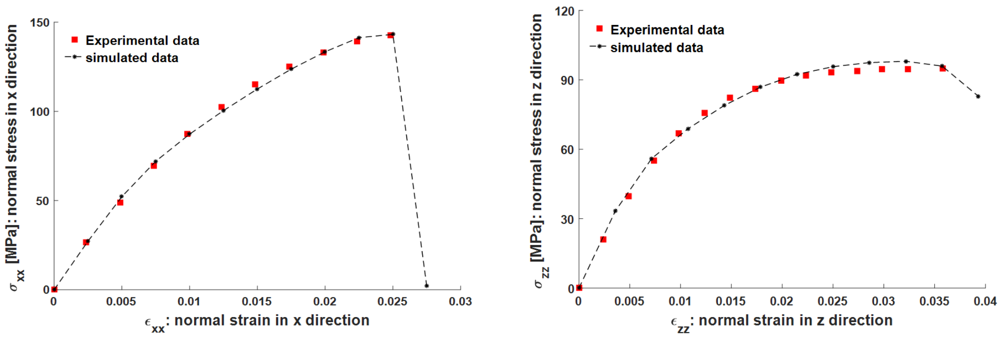

Рис. 5: Stress-strain response in DAM (left) and MC (right) samples as obtained in simulations and experiments

where the crack is localized in a single layer of elements. On the other hand, the damage pattern is much more diffuse in MC samples.

3. Conclusion

In the present manuscript, we present a multiscale approach for simulating degradation of composite structures in two environments: cyclic loading and exposure to humidity. For the carbon-fiber/epoxy-resin material system, we generalized the cycle block scheme to account for hybrid brittle-ductile failure. A reduced-order homogenization (ROH) approach is adopted for the prediction of damage accumulation in various microphases. For the glass-fiber/Nylon material system exposed to moisture we generalized the Fickian diffusion model [12] to account for the reaction of Nylon with water. The diffusion-reaction and mechanical problems were assumed to be two-way coupled where Nylon absorbed by water affects the mechanical behavior, while the damage accumulation is enhanced by the diffusion process of water. A first-order computational homogenization (FOCH) is employed for both diffusion-reaction and mechanical problems.

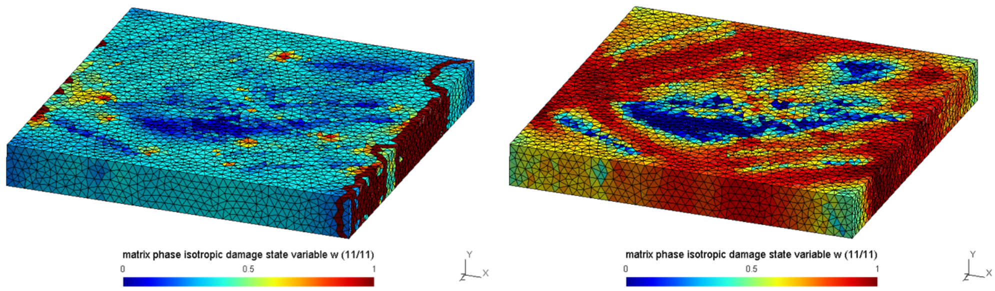

Рис. 6: The distribution of damage state variable in DAM (left) and MC (right) samples

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СПИСОК ЦИТИРОВАННОЙ ЛИТЕРАТУРЫ

1. Gerard, B., G. Pijaudier-Cabot, and C. Laborderie, Coupled diffusion-damage modelling and the implications on failure due to strain localisation. International Journal of Solids and Structures. International Journal of Solids and Structures, 35(31-32): p. 4107-4120.

2. Gerard, B., C. Le Bellego, and O. Bernanrd, Simplified modelling of calcium leaching of concrete in various environment. Materials and Structures, 2002. 35: p. 632-640.

3. Ulm, F.J., E. Lemarchand, and F. Heukamp, H., Elements of chemomechanics of calcium leaching of cement-based materials at different scales. Engineering Fracture Mechanics, 2003. 70: p. 871-889.

4. Terada, K. and M. Kurumatani, Two-scale diffusion–deformation coupling model for material deterioration involving micro-crack propagation. International Journal for Numerical Methods in Engineering, 2010. 83(4): p. 426-451.

5. Q. Yu and J. Fish, Multiscale asymptotic homogenization for multiphysics problems with multiple spatial and temporal scales: a coupled thermo-viscoelastic example problem, International journal of solids and structures 39 (26), 6429-6452, 2002

6. Kuznetsov, S. and J. Fish, Mathematical homogenization theory for electroactive continuum. International Journal for Numerical Methods in Engineering, 2012. 91(11): p. 1199-1226.

7. D. Klepach and T.I. Zohdi. Modeling and simulation of deformation-dependent diffusion in composite media. Composites Part B: Engineering. Volume 56, 413-423, 2014

8. T.I Zohdi and P. Wriggers. Introduction to computational micromechanics. Second Reprinting. Springer-Verlag., 2008.

9. T.I. Zohdi. An adaptive-recursive staggering strategy for simulating multifield coupled processes in microheterogeneous solids. The International Journal of Numerical Methods in Engineering. 53, 1511-1532, 2002.

10. T.I. Zohdi. Modeling and simulation of a class of coupled thermo-chemo-mechanical processes in multiphase solids. Computer Methods in Applied Mechanics and Engineering. Vol. 193/6-8 679-699, 2004.

11. M. Bailakanavar, J. Fish, V. Aitharaju and W. Rodgers, Coupling of moisture diffusion and mechanical deformation in polymer matrix composites Volume 98, Issue 12, pages 859–880, 2014.

12. R.J. Atkin and R.E. Craine. Continuum theories of mixtures: basic theory and historical development. Q.J. Mechanics Appl. Math., 29(2), 209–244, 1976.

13. R.M. Bowen. Theory of mixture. Continuum Physics III, 1–127, 1976.

14. R. Dunwoody. A thermomechanical theory of diffusion in solid-fluid mixtures. Arch. Ration. Mech. Anal. 38, 348–371, 1970.

15. K. Hutter and K. Jöhnk. Continuum Methods of Physical Modeling. Springer, Berlin, 2004

16. S. Lustig, J. Caruthers and N. Peppas. Continuum thermodynamics and transport theory for polymer-fluid mixtures. Chem. Eng. Sci., 47, 3037–3057, 1992.

17. I. Müller. A thermodynamic theory of mixtures of fluids. Arch. Ration. Mech. Anal. 28, 1–39, 1968.

18. N. Quang, I. Samohýl and H. Thoang. Irreversible (rational) thermodynamics of mixtures of a solid substance with chemical reacting fluids. Collect. Czech. Chem. Commun. 53, 1620–1635, 1988.

19. I. Samohýl and X.N.M. Šípek. Irreversible (rational) thermodynamics of fluid-solid mixtures. Collect. Czech. Chem. Commun. 50, 2346–2363, 1985.

20. C. Truesdell C. Mechanical basis of diffusion. J. Chem. Phys. Vol. 37, pp. 2336–2344, 1962.

21. V. Aitharaju, W. Rodgers, Internal General Motors Report, 2010.

22. H. K. Reimschuessel, "Relationships on the effect of water on glass transition temperature and young's modulus of nylon 6," J. Polym. Sci. Polym. Chem. Ed., vol. 16, no. 6, pp. 1229–1236, Jun. 1978.

23. J. Fish, Practical Multiscaling, Wiley 2013

24. Z. Yuan and J. Fish. Hierarchical model reduction at multiple scales. Hierarchical Model Reduction at Multiple Scales,"International Journal for Numerical Methods in Engineering, Vol. 79, Issue 3, pp. 314–339, (2009)

REFERENCES

1. Gerard, B., G. Pijaudier-Cabot, and C. Laborderie, 1998, Coupled diffusion-damage modelling and the implications on failure due to strain localisation. International Journal of Solids and Structures. *International Journal of Solids and Structures*, 35(31-32): p. 4107-4120.

2. Gerard, B., C. Le Bellego, and O. Bernanrd, 2002, Simplified modelling of calcium leaching of concrete in various environment. *Materials and Structures*, 35: p. 632-640.

3. Ulm, F.J., E. Lemarchand, and F. Heukamp, H., 2003, Elements of chemomechanics of calcium leaching of cement-based materials at different scales. *Engineering Fracture Mechanics*, 70: p. 871-889.

4. Terada, K. and M. Kurumatani, 2010, Two-scale diffusion–deformation coupling model for material deterioration involving micro-crack propagation. *International Journal for Numerical Methods in Engineering*, 83(4): p. 426-451.

5. Q. Yu and J. Fish, 2002, Multiscale asymptotic homogenization for multiphysics problems with multiple spatial and temporal scales: a coupled thermo-viscoelastic example problem, *International journal of solids and structures* 39 (26), 6429-6452,

6. Kuznetsov, S. and J. Fish, 2012, Mathematical homogenization theory for electroactive continuum. *International Journal for Numerical Methods in Engineering*, 91(11): p. 1199-1226.

7. D. Klepach and T.I. Zohdi. 2014, Modeling and simulation of deformation-dependent diffusion in composite media. *Composites Part B: Engineering.* Volume 56, 413-423,

8. T.I Zohdi and P. Wriggers, 2008, Introduction to computational micromechanics. Second Reprinting. Springer-Verlag.,

9. T.I. Zohdi. An adaptive-recursive staggering strategy for simulating multifield coupled processes in microheterogeneous solids. *The International Journal of Numerical Methods in Engineering*. 53, 1511-1532, 2002.

10. T.I. Zohdi. 2004, Modeling and simulation of a class of coupled thermo-chemo-mechanical processes in multiphase solids. *Computer Methods in Applied Mechanics and Engineering.* Vol. 193/6-8 679-699,

11. M. Bailakanavar, J. Fish, V. Aitharaju and W. Rodgers, 2014, *Coupling of moisture diffusion and mechanical deformation in polymer matrix composites Volume 98*, Issue 12, pages 859–880,

12. R.J. Atkin and R.E. Craine, 1976, Continuum theories of mixtures: basic theory and historical development. *Q.J. Mechanics Appl. Math.*, 29(2), 209–244,

13. R.M. Bowen, 1976, *Theory of mixture. Continuum Physics III*, 1–127,

14. R. Dunwoody, 1970, A thermomechanical theory of diffusion in solid-fluid mixtures. *Arch. Ration. Mech. Anal.* 38, 348–371,

15. K. Hutter and K. Jöhnk, 2004, *Continuum Methods of Physical Modeling.* Springer, Berlin,

16. S. Lustig, J. Caruthers and N. Peppas, 1992, Continuum thermodynamics and transport theory for polymer-fluid mixtures. *Chem. Eng. Sci.*, 47, 3037–3057,

17. I. Müller, 1968, A thermodynamic theory of mixtures of fluids. *Arch. Ration. Mech. Anal.* 28, 1–39,

18. N. Quang, I. Samohýl and H. Thoang, 1988, Irreversible (rational) thermodynamics of mixtures of a solid substance with chemical reacting fluids. *Collect. Czech. Chem. Commun.* 53, 1620–1635

19. I. Samohýl and X.N.M. Šípek, 1985, Irreversible (rational) thermodynamics of fluid-solid mixtures. *Collect. Czech. Chem. Commun.* 50, 2346–2363,

20. C. Truesdell, 1962, C. Mechanical basis of diffusion. *J. Chem. Phys.* Vol. 37, pp. 2336–2344,

21. V. Aitharaju, W. Rodgers, 2010, *Internal General Motors Report*

22. H. K. Reimschuessel, 1978, “Relationships on the effect of water on glass transition temperature and young’s modulus of nylon 6,” *J. Polym. Sci. Polym. Chem. Ed.*, vol. 16, no. 6, pp. 1229–1236, Jun.

23. J. Fish, 2013, *Practical Multiscaling*, Wiley

24. Z. Yuan and J. Fish, 2009, Hierarchical model reduction at multiple scales. Hierarchical Model Reduction at Multiple Scales, *International Journal for Numerical Methods in Engineering*, Vol. 79, Issue 3, pp. 314–339

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