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콘크리트 및 복합재료용 멀티스케일 가상 시험기계에 관한 소고

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Multiscale Virtual Testing Machines of Concrete and Other Composite Materials: A Review

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Abstract

Recently composite materials have dominated most engineering fields, owing to their better performance, increased durability and flexibility to be customized and designed for a specific required property. This has given them unprecedented superiority over conventional materials. With the help of the ever increasing computational capabilities of computers, researchers have been trying to develop accurate material models for the complex and integrated properties of these composites. This has led to advances in virtual testing of composite materials as a supplement or a possible replacement of laboratory experiments to predict the properties and responses of composite materials and structures. This paper presents a review on the complex multi-scale modelling framework of the virtual testing machines, which involve computational mechanics at various length-scales starting with nano-mechanics and ending in structure level computational mechanics, with a homogenization technique used to link the different length scales. In addition, the paper presents the features of some of the biggest integrated virtual testing machines developed for study of concrete, including a multiscale modeling scheme for the simulation of the constitutive properties of nanocomposites. Finally, the current challenges and future development potentials for virtual test machines are discussed.

Keywords : *virtual testing machines, concrete modeling, multiscale modeling, composites*

1. Introduction

In recent years, computer-aided modeling and simulation of engineering materials has emerged as a tool in the field of computational mechanics to understand and predict the mechanical properties of structures(Oden *et al.*, 2003). The progress in the computational capabilities of computers seems to fuel the advancement of material technology and engineering as it reduces the computational effort and time required for analysis(Okereke *et al.*, 2014). This modeling capability further enhanced material knowledge and innovation by facilitating the simulation of laboratory experiments which are difficult if not impossible to conduct. Furthermore, it has made possible the design and manufacturing of novel materials such as cellular materials, fiber reinforced polymer composites(FRPs) and concrete with different inclusions such as nanoparticles and carbon nano-tubes for enhanced performance(Llorca *et al.*, 2011; Okereke *et al.*, 2014; Yang *et al.*, 2014; Ha *et al.*, 2009; Ahn and Ha, 2017). In the past three decades, computational mechanics has achieved significant success in revolutionizing science and technology by

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using and modifying the principles of mechanics as a tool to predict and understand complex systems(Oden *et al.*, 2003). Computational mechanics being an interdisciplinary field mainly owes its success in impacting the numerous fields of science and technology to the progress in micromechanics and the drastic advancement in the field of computer science, which removed the manual computational effort(Okereke *et al.*, 2014). This helped to focus the research manpower on discovering modeling strategies to best simulate the physical matter under study by formulating mathematical models, algorithms and selecting appropriate initial and boundary conditions(Oden *et al.*, 2003). This paper reviews the complex multi-scale modelling framework of the virtual testing machines, which involve computational mechanics at various length-scales starting with nano-mechanics and ending in structure level computational mechanics, with a homogenization technique used to link the different length scales.

2. Virtual testing machines

2.1 What is virtual testing?

Virtual tests or virtual experiments are computer simulations that are sufficiently realistic enough to give the same results as actual laboratory tests(Cox and Yang, 2006). Virtual tests present tremendous savings in testing labor costs and material design cycle times. Besides these, virtual testing presents three advantages over physical laboratory experimentation of composite materials(Bentz, 1997). First, any complex loading mode can be applied to the composite structure with minimal computational efforts. Secondly, virtual testing makes the analysis and study of the progressive damage in composites relatively simpler, and finally the effect of phase distribution and micro constituent parameters on the properties of composite can be investigated with relative ease(Bentz, 1997).

Virtual testing has been gaining large popularity in the fields of composite materials due to its large economical advantage(Gonzalez and LLorca, 2007). This review will focus on describing the basic steps of the virtual experimental setups and the role it will play in the future of composite material engineering.

2.2 Components of a multiscale virtual experiment

The setup and focus of investigation of a virtual experiment for composite materials generally depends on the problem being studied. The effective properties of composite materials that influence the macro-structural properties and require in-depth study with virtual testing or numerical modeling are volume fraction of the inclusions, their spatial distribution in the composite matrix and the properties of the phases and interfaces(Okereke *et al.*, 2014). Meanwhile, other researchers argue that in order to design composite materials, understanding the complex damage and failure propagation properties is the most critical and challenging part(Cox and Yang, 2006).

The general strategy for virtual testing of composites consists of defining the virtual problems of the domain of interest(Okereke *et al.*, 2014). This is accomplished by defining the boundary or geometry within which the material being investigated exists, which is the representative volume element(RVE for 3D composites or representative cell element(RCE) for 2D composites)(Qu and Cherkaoui, 2006). After this, one should define the nature of the declared virtual domain: elastic or inelastic, linear or non-linear. This step constitutes the selection and application of a series of mathematical and micromechanical models and based on the microstructure of the material such as constitutive models for unidirectional laminated composites(Liang *et al.*, 2006), models for characterization of the progressive damage in composites(Lee *et al.*, 2008). It is essential that the development of the microstructure appropriately considers the innate material characteristics such as the material symmetry, homogeneity, heterogeneity and the spatial distribution of the constituents in the microstructure.

After the constitutive equations are properly defined,

the virtual test machine then applies the appropriate boundary conditions on the defined virtual domain to determine the response(stress strain relations) of the virtual domain, either using homogenization techniques (Charalambais, 2017) or directly from the virtual experimental response, depending on the length scale the test machine is working on. Last but not least, the last step consists of validation of the results from the virtual experiments, which can be done by comparing the results from the virtual experiment with physical experimental responses(Akpoyomare *et al*., 2017).

The major computational tools that are playing the biggest roles in the advancements of virtual testing and mulit-scale simulation are quantum mechanics, density functional theory, standard and coarse grained molecular dynamics, Monte-carol methods of kinetics, computational thermodynamics, phase field modeling, dislocation dynamics, large family of partial differential equation solvers(FEM and finite difference methods), damage mechanics, micromechanics and homogenization theories that link the different length scales(Llorca *et al*., 2011; Charalambais, 2017). Besides the above stated strategies, the other key issue in virtual testing is the huge length-scale that has to be bridged when trying to model composite materials(Okereke *et al*., 2014).

2.3 Length scales in virtual testing

Virtual testing must incorporate the multiscale approach in order to represent full laboratory scale experiments, since engineering material properties such as stiffness, strength and toughness depend on different factors that exist in different length scales (Okereke *et al*., 2014). Therefore, the numerical modeling must start with the smallest functional unit, usually nanoscale for engineering material purposes, and proceed to microscale, mesoscale and finally macroscale. And it can be inferred that the computational method the virtual experiments must employ in each step varies accordingly(Llorca *et al*., 2011).

3. Some virtual laboratories and their features

The three-dimensional computer simulation of cement, concrete and other composites is not a recent development. Perhaps considered as pioneers, Wittmann *et al*.(1984~1985) made the earliest attempts to represent the microstructure of concrete numerically on a computer(Bentz. 1997). Right about the same time, Jennings and Johnson(1986) simulated the hydration of cement by modeling the cement particles as spheres made of tricalcium silicate(C_3S), whereby the hydrated gel, calcium silicate hydrate(C-S-H), surrounds these spheres and the width of this gel increases as the hydration time progressed(Bentz, 1997). Other researchers such as Bentz *et al*. developed 3D computer models that simulate the hydration of cement and the development of concrete microstructure in the late 1990s.

Following these, several studies have been conducted in order to push this research field into developing integrated simulation schemes that resemble the current virtual testing machines. A general outline of a virtual testing scheme for composite materials was outlined by Okereke *et al*.(Okereke *et al*., 2014).

While the above researches focused on modeling a specific type of fiber and specific area for the virtual experiments(Okereke and Akpoyomare, 2013; Okereke. *et al*., 2008), some large scale virtual laboratories have been developed by different researchers. Some of these virtual laboratories are developed to study the micro-macro mechanical properties of concrete, by simulating the different degrees of cement hydration (Bernard and Lemarchand, 2003), aggregate properties and the properties of the interfacial transition zone (Nilsen, 1993; Ishida *et al*., 2005).

3.1 Virtual Test Facility(VTF) at Caltech Center

Developed as a test facility that utilizes time-explicit numerical methods in order to simulate the dynamic response of materials, the Virtual test facility

(VTF) was designed to simulate the dynamic response of materials(California Institute of technology, 2017). This facility is a synergy of computational engines compiled and driven together by a user interface that is responsible for most aspects of the simulation, such as the geometry generation, material selection and visualization of the outputs(Aivazis *et al*., 2000). The virtual machine is an open source software that uses python scripting language for the code(Aivazis *et al*., 2000). The virtual test facility has three main modules, AMROC- which is a finite volume fluid solver that uses Eulerain framework, SFC- a thin-shell finite element solid solver that uses Lagrangian computation and STLIB- an assemblage of templatized auxiliary algorithms(Okereke *et al*., 2008).

By the coupling action of these modules, the VTF is capable of simulating fluid-structure interaction problems which are profoundly coupled and the fragmentation and rupture of brittle materials under shock wave impact(Okereke *et al*., 2008).

3.2 Virtual Cement and Concrete Testing Laboratory(VCCTL)

The advancement in the simulation tools for cement and concrete at micro and mesoscales(micrometers and millimeters respectively) has made possible the fast progress of the virtual testing laboratories with the aim of reducing the number of physical test, quality assurance and speeding up the research process(Bentz, 1997). One of these virtual testing laboratory packages is the Virtual Cement and Concrete Testing Laboratory(VCCTL), which is an integrated software package developed by a consortium of researchers led by the National Institute of Standards and Technology(NIST), USA(Bullard *et al*., 2009). The VCCTL is developed to aid in the material selection, design and optimization process of construction materials, mainly concrete(Bullard *et al*., 2009).

The VCCTL has been available for commercial use since 2000, with the release of its first version, Version 1.0 and Version 9.5 being released in 2014. VCCTL developed as software, allows the creation of a 3D RVE of the cement microstructure based upon the 3D representation of the microstructure from several digital-images(Okereke *et al*., 2013). It then simulates the hydration of the RVE under any curing condition and allows the analysis for properties of the materials such as elastic moduli, compressive strength and relative diffusion coefficients etc.(Bentz, 1997; Okereke *et al*., 2013).

The main features of VCCTL include having a wide database of cement, aggregates, fly ash, slag and inert fillers(Bullard *et al*., 2009). It can simulate the hydration of the microstructure for a prescribed time, and displays the hydration results(Bullard *et al*., 2009). It also calculates the elastic properties of hydrated cement, mortar and concrete. Moreover, it is able to predict the diffusion coefficient of hydrated cement, while allowing visualization of the 3D microstructure of the concrete including the pore size distribution(Bullard *et al*., 2009).

3.3 DuCOM, COM3 and WCOMD: Durability models of concrete

The Durability Models for Concrete(DuCOM), COM3 and WCOMD(originally non-commercial modeling software) were developed in the early 2000s in the concrete laboratory at Tokyo University(Ishida *et al*., 2005). These virtual laboratories' ultimate objectives are the simulation of the nonlinear mechanical response of concrete structures(COM3 and WCOMD, structure level multi-scale simulators) and the simulation of the life span of concrete(DuCOM), which the developers referred to as "life-span simulator" of structural concrete(Ishida *et al*., 2005). It incorporates micro-scopic modeling of concrete along with the precise implementation of the many physio-chemical processes that act on it(Ishida *et al*., 2005).

Focusing on the material simulator DUCOM, the developers of this computational platform used a thermo-dynamic modeling approach by considering the micro-scale pores in concrete as growing in time(Maekawa *et al*., 2003). This dynamic pore

Table 1 Comparison of the virtual testing facilities in literature

	VCCTL Bullard,(2009)	**VTF** Deiterding,(2006)	**DuCOM** Ishida,(2005)
Realistic spatial representation			
Specimen geometry	- 3D-digital image representation of concrete microstructure	- Disjointed fluid, solid domains and interaction occurs only at the fluid-solid interface.	- Microstructural modeling of concrete, user defines the structure geometry
Material dataset	- Cement, aggregates, mineral admixtures	- Has extensive VTF material Library	- Works for cement and the different pozzolanic powders (allows for the user input)
Relevant boundary conditions			
Load case and periodic boundary condition	- Curing condition(isothermal, adiabatic, variable evaporation rate)	- Lagrangian and Eulerian element schemes to model the boundary conditions	- Defined by the user in terms of history of structure's exposure to the environment.
Computational material models			
Linear and nonlinear deformation Failure process Continuum and non-continuum damage	- Lab material module - Mix proportion module - Curing Module: different thermal conditions - Measurements module, - Uses CEMHYD3D: cement hydration	- SFC: Lagrangian thin shell finite element), - AMROC: Eulerian finite volume fluid solver - STLIB: a collection of auxiliary algorithms(Aivazis *et al.*, 2000)	- Mono-sized particle dispersion and expansion model - Moisture transport model: multi-component porosity - Thermo-dynamic hydration model:(Maekawa *et al.*, 2003)
Testing Platform			
	- Online VCCTL server based software	- Python scripting layer - A combination of more than five computational solvers	- Fortran codes - DuCOM FEM solver
Final predicted properties			
	- Degree of hydration, chemical shrinkage, pore percolation, diffusivity, elastic moduli, - Strength development,	- Determines response of solid and fluid structures to dynamic loads, peak stresses and stress concentrations	- Long term durability: Deterioration, thermal cracks, chemical processes, rebar corrosion, shrinkage and creep - Short term durability
Software type			
	- Commercial(2000)	- Open source	- Now commercially available
Strongest point			
	- Wide material data base - Concrete optimization and design	- Modeling the dynamic fluid-structure interaction efficiently	- Its multi-scale capability
Efficiency			
Computation time and cost	- It is a web server application so computational demand on a PC is small.	- Uses explicit-time integration which is computationally expensive	- The interdependency of different physical phenomenon's can be taken into account.
Code and interface ease (subroutines)	- User friendly and easy to input new material data	- ~430,000 lines of code	- User friendly(no information on adding user subroutines)

growth will affect the major mechanical and physical characteristics of concrete and its long term durability, which the simulation must incorporate. DuCOM integrates the early stage hydration, microstructure formation and moisture transport processes of concrete into its algorithm(Maekawa *et al.*, 2003).

The DuCOM simulation framework consists of three modules(Ishida *et al.*, 2005). The first is the microstructure development, which utilizes a dispersion of a single sized particles and particle expansion model (Ishida *et al.*, 2005). The second module is a moisture transport model that is based on the multi-component division of concrete space porosity, that can be used for any path of drying and wetting (Ishida *et al.*, 2005). The third module consists of a hydration model, which utilizes a multi-component division of cement and pozzolanic powder materials (Ishida *et al.*, 2005). Based on the modified Arrhenius's

law, it obtains the rate of heat generation for each of these components(Ishida *et al*., 2005). The simulation scheme begins from the casting of concrete and follows the developments of strength, porosity and pore moisture content history with time(Ishida *et al*., 2005).

Table 1 shows a brief but comparative observation of the three virtual testing facilities discussed above. Considering the difference in the general aims and goals of the software, the comparison is made in a more of explanatory manner. This is essential as comparing the computation time, cost and other parameters of a multiscale model and a single level analysis will not be practical.

3.4 A multiscale modeling scheme for the constitutive property determination of nanocomposites

All virtual testing laboratories do not have to be compiled software packages as we have seen in the cases above. In fact, what makes virtual testing laboratories so attractive for the future is the ability for small number of researchers to collaborate and develop their own virtual laboratories that can be geared towards investigating in detail some specific properties of complex materials, such as interfacial properties.

A case in point is a multiscale modeling scheme proposed by Yang *et al*., 2013, that is composed of molecular dynamics(MD), micromechanics, and finite element modeling(FEM) tools in order to determine the interfacial effects of nanocomposites(Yang *et al*., 2013). The primary motivation behind the developed scheme was, as the classical continuum mechanics and composite theory cannot fully and accurately account for the mechanical behavior of nanocomposites, to utilize the combined tools of MD simulation techniques and the classical micromechanics method for the estimation of the interfacial effect of nano-inclusions in a matrix(Yang *et al*., 2013). The interfacial property is particularly important in nanocomposites because the interfacial contact area between the inclusions and the matrix is dramatically widened as compared with the conventional composite material(Jordan *et al*., 2005; Zhu. *et al*., 2005).

Hence, the contents of the above mentioned multiscale modeling scheme are as follows. First, the ensemble volume averaging method based micromechanical model is proposed that takes into account the characteristics of the interface(Lee, 2001; Yang *et al*., 2013). Since there is no clear way of determining interfacial moduli in the proposed micromechanics-based constitutive equation, the scheme uses MD simulation to determine the bulk modulus of the nanocomposite which it will cross check with the micromechanics parametric study of the bulk modulus(Yang *et al*., 2013). Therefore, after cross checking this, the model determines the accurate values for the interfacial moduli and uses the micromechanics model to determine the constitutive matrix C^* for the nanocomposite material (Yang *et al*., 2013). The significance of the study is that the results are derived purely through computational analysis without additional fitting process.

After this, the multiscale modeling scheme goes on to determine the macroscale properties for the nanocomposite by inputting the constitutive material property values into the finite element(FE) software, ABAQUS. For more detail on the scheme, refer to the paper(Yang *et al*., 2013). Finally, using the FE tool, the scheme is able to predict accurately the elastic response of the nanocomposite up to the yielding point. However, since the micromechanics method applied for this scheme only works for the elastic range, further work is required to make the multiscale model more inclusive and general.

4. Challenges of virtual testing and the future prospect

Several researchers have stated that virtual testing is the future of composite material engineering that has the potential to transform the material engineering industry tremendously(Oden, 2003, Okereke *et al*., 2014, Bullard *et al*., 2009). However, several

challenges still need to be overcome for the multi-scale virtual simulation of composites to reach the reliability level of physical laboratory experiments.

The first challenge is the difficulty in developing an accurate geometric, micromechanical and multiscale material model(Okereke *et al*., 2014). Overcoming the challenge of either using a tomographic based image reconstruction or using topological parameters to construct regularized numerically generated RVEs is vital(Okereke *et al*., 2014). Another method is relaying on molecular dynamics models, another simulation tool, which can reconstruct molecular and nano-structures of a crystal of the material in order to develop the RVE(Yang *et al*., 2013). Second, the choice of appropriate boundary conditions based on the simulation scheme and assumptions affects the accuracy of the virtual experiments. Next, the development of robust homogenization techniques that assist the transfer of the obtained properties up the length scale without the smearing of the responses is another topic that requires further study(Oden, 2003). Finally, the validation of numerical predictions with experimental data presents the biggest challenge for virtual testing, as some of the virtual experiments cannot be exactly performed in physical experiments(Oden, 2003; Okereke *et al*., 2014).

5. Concluding remarks

As presented above, a multiscale virtual testing platform presents the fields of material science and computational mechanics an incredibly versatile and useful tool that reduces the analysis, design and production time when working with new and complex composite materials. The major advantages of these multiscale virtual testing machines include the relative ease with which complex geometries, loading conditions and material properties can be modeled and analyzed, how they provide researchers the ability to zoom into the composite material properties to investigate complex failure mechanism such as progressive damage modeling and how the study of complex composite materials such as cementitious composite with different phases and inclusions can be investigated in a relatively better way(Bentz, 1997).

In order for virtual testing to work as supplement or replacement of physical laboratory experiments, virtual laboratories' framework must match analogously the physical laboratories' framework(Okereke *et al*., 2014). This requires that virtual testing follow a multiscale modeling approach where the virtual laboratory must incorporate the different levels of computational mechanics and link these levels by using a proper homogenization technique to transfer the information of the material from one length scale level to another. For virtual testing to utilize its full capacity, it requires that still unsolved issues such as developing an appropriate boundary condition, development of vigorous homogenization schemes and the difficulty of acquiring sufficient data for validation of the created models be further investigated and resolved(Okereke *et al*., 2014).

The other important issue that should be considered when thinking of multiscale virtual testing machines is the issues related to its core principle that is the multiscale modeling scheme. This scheme by itself comes with unresolved concerns related to the model validation, the appropriateness of the length scale bridging techniques and error propagation when traversing across the different length scales(Hoekstra *et al*., 2013). Some ground breaking work has been done by Oden *et al*.(2006) with regards to the controlling and quantifying the error propagation in the multiscale modeling, which shades some light on the importance of the issue. However, there is still a large knowledge gap to fill. Hence, this presents future researchers in the field of computational mechanics and materials engineering a vast possibility of simulation research areas, where the understanding of these complex materials can be remarkably improved.

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References

Ahn, T.S., Ha, Y.D. (2017) Study on Peridynamic Interlayer Modeling for Multilayered Structures, *J. Comput. Struct. Eng. Inst. Korea,* 30(5), pp.389~396.

Aivazis, M., Goddard, W.A., Meiron, D., Ortiz, M., Pool, J., Shepherd, J. (2000) A Virtual Test Facility for Simulating Thermodynamic response of Materials, *Comput. Sci. & Eng.*, 2(2), pp.42-53.

Akpoyomare, A.I., Okereke, M.I., Bingley, M.S. (2017) Virtual Testing of Composites: Imposing Periodic Boundary Conditions on General Finite Element Meshes, *Compos. Struct.*, 160(15), pp.983~994.

Bentz, D.P. (1997) Three-Dimensional Computer Simulation of Portland Cement Hydration and Microstructure Development, *J. Am. Ceram. Soc.*, 80(1) pp.3~21.

Bernard, O., Ulm, F., Lemarchand, E. (2003) A Multiscale Micromechanics-Hydration Model for the Early-age Elastic Properties of Cement-Based Materials, *Cement & Concr. Res.*, 33(9), pp.1293~1309.

Bullard, J.W. (2016) *Virtual Cement and Concrete Testing Laboratory: Version 9.5 User Guide*, National Institute of Standards and Technology, Special Publication SP 1173, p.60.

Bullard, J.W., Stutzman, P.E., Belloc, L.M.O., Garboczi, E.J., Bentz, D.P. (2009) *Virtual Cement and Concrete Testing Laboratory for Quality Testing and Sustainability of Concrete*, National Institute of Standards and Technology, Special Publication SP 266. pp.27-36.

California Institute of Technology (2017) The Virtual Test Facility, VTF. Retrieved from http://www.vtf.website/asc/wiki/bin/view/

Charalambakis, N. (2010) *Homogenization Techniques and Micromechanics*, A Survey and Perspectives, Applied Mechanics Reviews, 63, pp.1-10.

Chong, K.P., Garboczi, E. (2002) Smart and Designer Structural Material System, *Prog. Struct. Eng. Mater.*, 4(4), pp.417-430.

Cox, B., Yang, Q. (2006) In Quest of Virtual Tests for Structural Composites, *Sci.*, 314(5802), pp.1102~1107.

Deiterding, R. Radovitzky, R. Mauch, S.P., Noels, L, Cummings, J.C., Meiron, D.I (2006) A Virtual Test Facility for the Efficient Simulation of Solid Material Response under Strong Shock and Detonation Wave Loading, *Eng. Comput.*, 22(3-4) pp.325~347.

González, C., LLorca, J. (2007) Virtual Fracture Testing of Composites: A Computational Micromechanics Approach, *Eng. Fract. Mech.*, 74(7), pp.1126~1138.

Ha, S.K., Yang, B.J., Lee, H.K., (2009) Finite Element Analysis for Evaluating the Performance of RC Beams Strengthened with SFRP Coating, *J. Comput. Struct. Eng. Inst. Korea*, 22(6), pp.579~585.

Hoekstar A., Chopard B., Coveney, P. (2014) Multiscale Modeling and Simulation: A Position Paper, *Phil. Trans. R. Soc.*, A372, 20130377.

Ishida, T., Tsuchiya, S., Chaube, R.P. (2005) "DUCOM DEMO" (August 2, 2017) Retrieved from http://concrete.t.u-tokyo.ac.jp/en/demos/ducom/.

Jennings, H.M., Johnson, S.K. (1986) Simulation of Microstructure Development during the Hydration of a Cement Compound, *J. Am. Ceram. Soc.*, 69(11), pp.790~795.

Jordan, J., Jacob, K.I., Tannenbaum, R., Sharaf, M.A., Jasiuk, I. (2005) Experimental trends in polymer nanocomposites-a review, Materials Science and Engineering. A 393, 1.

Lee, H.K., Pyo, S.H. (2008) Multi-Level Modeling of Effective Elastic Behavior and Progressive Weakened Interface in Particulate Composites, *Compos. Sci. & Tech.*, 68(2), pp.387~397.

Lee, H.K. (2001) A Computational Approach to the Investigation of Impact Damage Evolution in Discontinuously Reinforced Fiber Composites, *Comput. Mech.*, 27(6), pp.504~512.

Liang, Z., Lee, H.K, Suaris, W. (2006) Micromechanics based Constitutive Modeling for Unidirectional Laminated Composites, *Int. J. Solids & Struct.*, 43(18-19), pp.5674~5689.

Llorca, J., González, C., Molina-Aldareguía, J. M., Segurado, J., Seltzer, R., Sket, F., Canal, L.P. (2011) Multiscale Modeling of Composite Materials: A Roadmap Towards Virtual Testing, *Adv. Mater.*, 23(44), pp.5130~5147.

Maekawa, K., Ishida, T., Kishi, T. (2003) Multi-scale Modeling of Concrete Performance Integrated Material and Structural Mechanics, *J. Adv. Concr. Technol.,* 1(2), pp.91~126.

Nilsen, A.U., Monteiro, P.J.M. (1993) Concrete: A Three Phase Material. Cement and Concrete Research, 23, pp.147~151.

Oden, J.T., Belytschko,T., Babuska, I., Hughes, T.J.R. (2003) Research Directions in Computational Mechanics, *Comput. Methods Appl. Mech. & Eng.*, 192(7-8), pp.913~922.

Oden, J.T., Prudhomme, S., Romkes, A., Bauman, P.T. (2006) Multiscale Modeling of Physical Phenomena: Adaptive Control of Models, *SIAM J. Scien. Comput.,* 28(6), pp.2359~2389.

Okereke, M., Petrinic, N., Wiegand, N., R. Gerlach., S.iviour, C. (2008) Virtual Testbed for Numerical Homogenization of Elastic Behavior and Damage Initiation in Bidirectional Composites, *Proceedings of Research: 8th World Congress on Computational Mechanics* (June30-July5, 2008) Italy, pp.1~3

Okereke, M.I., Akpoyomare, A.I. (2013) A virtual Framework for Prediction of Full-Field Elastic Response of Unidirectional Composites, *Comput. Mater. Sci.*, 70, pp.82~99.

Okereke, M. I., Akpoyomare, A. I., Bingley, M. S. (2014) Virtual Testing of Advanced Composites, Cellular Materials and Biomaterials: A Review, *Compos. Part B: Eng.,* 60, pp.637~662.

Qu, J., Cherkaoui, M. (2006) *Fundamentals of Micromechanics of Solids*, New Jersey: John Wiley & Sons, Inc., Hoboken.

Wittmann, F.H., Roelfstra, P.E., Sadouki. H. (1985) Simulation and Analysis of Composite Structures, *Mater. Sci. & Eng.,* 68(2), pp.239~248.

Yang, B.J., Ha, S.K., Lee, H.K. (2012) Micromechanics-based Analysis on Tensile behavior of the Sprayed FRP Composites with Chopped Glass Fibers, *J. Comput. Struct. Eng. Inst. Korea*, 25(3), pp.211~217.

Yang, B.J., Hwang, Y.Y., Lee, H.K. (2013) Elastoplastic Modeling of Polymeric Composites Containing Randomly Located Nanoparticles with an Interface Effect, *Compos. Struct.*, 99, pp.123~130.

Yang, B.J., Shin, H., Lee, H.K., Kim, H. (2013) A Combined Molecular Dynamics / Micromechanics / Finite Element Approach for Multiscale Constitutive Modeling of Nanocomposites with Interface Effects, *App. Phys. Lett.,* 103(24), 241903.

Zhu, L., Narh, K.A. (2004) Numerical Simulation of the Tensile Modulus of Nanoclay Filled Polymer Composites, *J. Polym. Sci. Part B: Polym. Phys.* 42(12), pp.2391~2406.

요 지

최근 복합재료는 향상된 성능, 내구성 및 여러 특정 요구성능에 대한 설계 유연성으로 인해 다양한 분야에서 활발히 활용되고 있다. 컴퓨터 성능이 발달함에 따라, 복합재료의 복잡한 거동에 대한 정확도 높은 모델 역시 함께 연구되고 있으며, 이로 인해 가상시험이 복합재료 거동에 대한 실험을 대체하거나 보충하는데 중요한 역할을 하고 있다. 본 논문에서는 나노수준부터 구조물 단위까지 이르는 다양한 length scale의 homogenization을 통한 멀티스케일 모델링에 대한 문헌을 분석하였다. 또한, 콘크리트 거동 연구에 대한 통합모델의 특징을 다루었으며, 가상 시험기계에 대한 최근 연구동향 및 전망에 대하여 다루었다.

핵심용어 : 가상 시험기계, 멀티 스케일 모델링, 복합 재료, 콘크리트 모델링