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## Build-up of new nature-mimicking materials using automated simulation routines—the future trend?

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The current consumption of fossil fuel resources and respective L production of traditional polyolefin plastics has led to huge clustering of plastics in oceans as well as in landfill sites. In its simplicity, sole recycling will never solve the waste problems because plastics will anyway be left unrecycled at a finite rate due to the human nature. Biodegradable, isotropic polymer blends are neither a complete solution for all applications because their performance is far behind that of current highperformance polymers, such as the ones of epoxy, vinylester, aramid, and bismaleimide thermoset families. Basically all the biodegradable polymeric systems for structural applications are continuous fibre-reinforced plastics. In these composites, either the reinforcement (e.g. bio-based fibres) or the polymer matrix is the degradable component. The reinforcing particles can have various forms and involve wood particles and fibres, natural fibres (e.g. flax or hemp), clay, starch, and cellulose. For high performance applications, the outcome of these studies boils down to the fact that there is always a distinctive compromise between a high bio-particle content and good mechanical properties, or, in other words, the composites represent a double-edged sword with some sustainability and mechanical performance. However, a carefully adjusted mixture of synthetic and natural fibres can result in a better mechanical response, e.g. against impact loads, compared to composites with only either type of reinforcement. Graphite as well as carbon nanotubes have excellent electrical, mechanical and thermal properties. For these reasons they are considered to be used in many types of composites in the future. Combining CNTs with cellulose has known to be eco-friendly, efficient, low cost and non-metal based option. Applications of CNT/cellulose composites usage are reported to be in the fields of electromagnetic interference shielding, chemical vapour sensors and in pressure sensing. Also, totally new species of advanced 'nat- ural' materials are being developed. For example, the nacre-mimetic materials are a type of nano-composite that significantly benefits the synergetic arrangement of its rather unique poly(vinyl alcohol)/clay building blocks. The maturity of these materials is on a laboratory level and will take long until their processing can reach commercial needs. Eventually, any environment degrades the material properties of polymeric systems. In order to create new high-performance composites, the degradation behavior must be understood and controlled.

Especially the fibrous composite materials are challenging to analyse considering the aging response. Even pure linear anisotropic models will require nine engineering constants per material not to mention the interface models to tie different layers together, or the internal residual stress models. The question from the numerical analysis point of view is how to define relevant parameters when modelling the environmental effects of laminate or an entire structure. This presentation will deal with the application of automated simulation routines to design new materials. Ex- amples of using Abaqus-Isight (Simulia) coupling are presented for understanding the aging in high-performance glass-fibre reinforced composites (Fig. 1(a)). The focus in these cases are on the challenges of building up the material model for a layered composite with correct interface models. In the second part of the presentation, examples of new materials with optimized nano-strengthening are presented (Fig. 1(b)). Film preparation using nanofibrillated cellulose, CNTs as well as electrospinning are described with emphasis on the sonication models, particle-ratios and de-hydration. The presentation will discuss the future trends in using autonomous and smart numerical simulations to screen most potential multicomposites for optimized behavior in specific applications.





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Figure 1: a) Stacked simulation routine description when using finite element methods (Abaqus/Isight) for understanding aging-effects on the flexural behavior of fibrous composite laminates. b) SEM imaging of an optimized material based on MWCNT network on a NFC surface.

## **Biography**

Professor (tenure track) Mikko Kanerva leads the research group of Plastics and Elastomer Technology in Tampere University of Technology, Laboratory of Materials Science. His group of 17 researchers focuses on the synthesis and modelling of polymer composite materials through the application fields of aerospace and the infrastructure. He has been teaching programmes such as Aircraft Structural Design, Composites, and Airline Transport Pilot training, for instance. Kanerva has completed his PhD from Aalto University. He serves as the representative of Finland for the International Council of the Aeronautical Sciences (ICAS) and its Programme Committee, Early Career Committee, and External Relations Committee.

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