

Modeling at Continental Tire - An Interview with Michael York

The website (www.continentaltire.com) of Charlotte, NC-based Continental General Tire Inc. reads, "For over 125 years, Continental Tires have been performing for some of the world's most famous automotive nameplates across the globe. Continental produces high performance, touring, highway and off-road tires for most of today's premium vehicles. Whether they drive a Porsche Boxster or a Lincoln Navigator, Continental has the size and the style that fits."

This leading automobile tire manufacturer have been using computational techniques in their R&D to provide understanding of chemical reaction phenomena and insight for refining the tire manufacturing process and tire performance.

The challenge faced

Michael York of Continental Tire was requested to assist in identifying current bladder life cycle restrictions and provide recommendations that would increase the number of cured tires per single curing bladder and augment daily curing production at their North American plants. Using computational chemistry, one year later York had characterized an anomaly due to an adverse reaction of materials during the bladder curing process and recommended mixing-procedure changes. These changes have generated an estimated saving of \$1.5 million per annum.

The interview

What follows is the transcript of an interview conducted by Accelrys with Michael York.

What modeling, simulation, and/or informatics software does your company use?

Cerius² and Materials Studio 2.0.

What do you use it for? How does this work fit in with your company's long-term goals?

Continental employs the use of molecular modeling to provide (1) knowledge and understanding of complex reaction mechanisms and observed chemical phenomena, (2) insight and direction for product innovation, and (3) solutions for reducing production costs.

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Have you published work in the scientific literature and/or general press that uses computational software? If so, when and where?

My work in materials science at Continental Tire North America is of a confidential nature. All papers and presentations containing computational chemistry are not available to the public at this time.

What did the software enable you to do that experimentation didn't?

Computational chemistry provides the total energy of any molecule real or imaginary. That information can not be determined in the laboratory. Consequently, it also provides certain thermodynamic data that relates to the spontaneity of a reaction, transition state structures, and rates of reactions. The chemist is not limited by laboratory capabilities or literature availability.

What would you say are the main scientific advantages of using computation over experimentation? Likewise financial advantages? Did its use save resources - i.e. time, money...?

Experimentation takes manpower, chemicals, equipment, energy, and time. Computational chemistry allows one operator to run multiple chemical reactions 24 hours a day. By performing the 'experiments' on the computer, the chemist can eliminate non-productive reaction possibilities and narrow the scope of probable laboratory successes. The end result is a major reduction in laboratory costs (materials, energy, equipment, etc.) and manhours.

How long would you say that it took for your company/organization to re-coup the initial investment in the software (including initial, installation and running costs) with any cost savings mentioned in the previous question?

Continental Tire was able to re-coup the initial investment in the software and hardware in less than 12 months.

Did the use of the computational chemistry techniques result directly in refinements to existing processes? And, if so, how much has it saved your company? And in the future?

Curing bladders are manufactured by compounding using a Banbury mixing process that involves time and temperature. The life span of these bladders is determined by the compounding formula and the time and temperature at which the ingredients are incorporated into the mix. Adverse reactions during the mixing process will shorten bladder life. A refinement in our process was directly initiated based on the knowledge and understanding gained from identifying the adverse reaction by modeling. A savings of over \$1.5 million per year was realized.

Did the use of the computational chemistry techniques allow you to gain a competitive advantage?

There are ongoing Continental Tire projects that are employing the use of molecular modeling to secure a competitive edge in the market place. One project involves bonding magnetic material into the sidewall of a tire, which produces a magnetic field for measuring wheel speed, brake torque, and lateral force. Metal does not naturally bond to rubber, therefore a new type coupling agent had to be designed. Computational chemistry was used to design a material with high affinity and specificity for the magnetic compound. The results were outstanding.

What do you and your organization plan to use the software for in the future?

Owing to the confidential nature of the work, I can not give any specifics of future projects. However, it is my opinion that as we increase our knowledge of computational methods and expand our capabilities of this software, Continental will broaden its utilization of the software into many other diverse arenas within the industry. This simulation tool is an integral part of our technical capabilities in atomistic, mesoscale, and continuum type modeling.

Would you recommend the use of modeling/simulation to your peers?

I highly recommend molecular modeling for research and material development; however, modeling is only as good as the scientist at the keyboard. If a company is willing to invest the time to learn the techniques and how to apply them, then this tool will be an exceptional asset for problem solving, product innovation, and cost reduction.