Tying Together Theory and Tests via Virtual Testing

by

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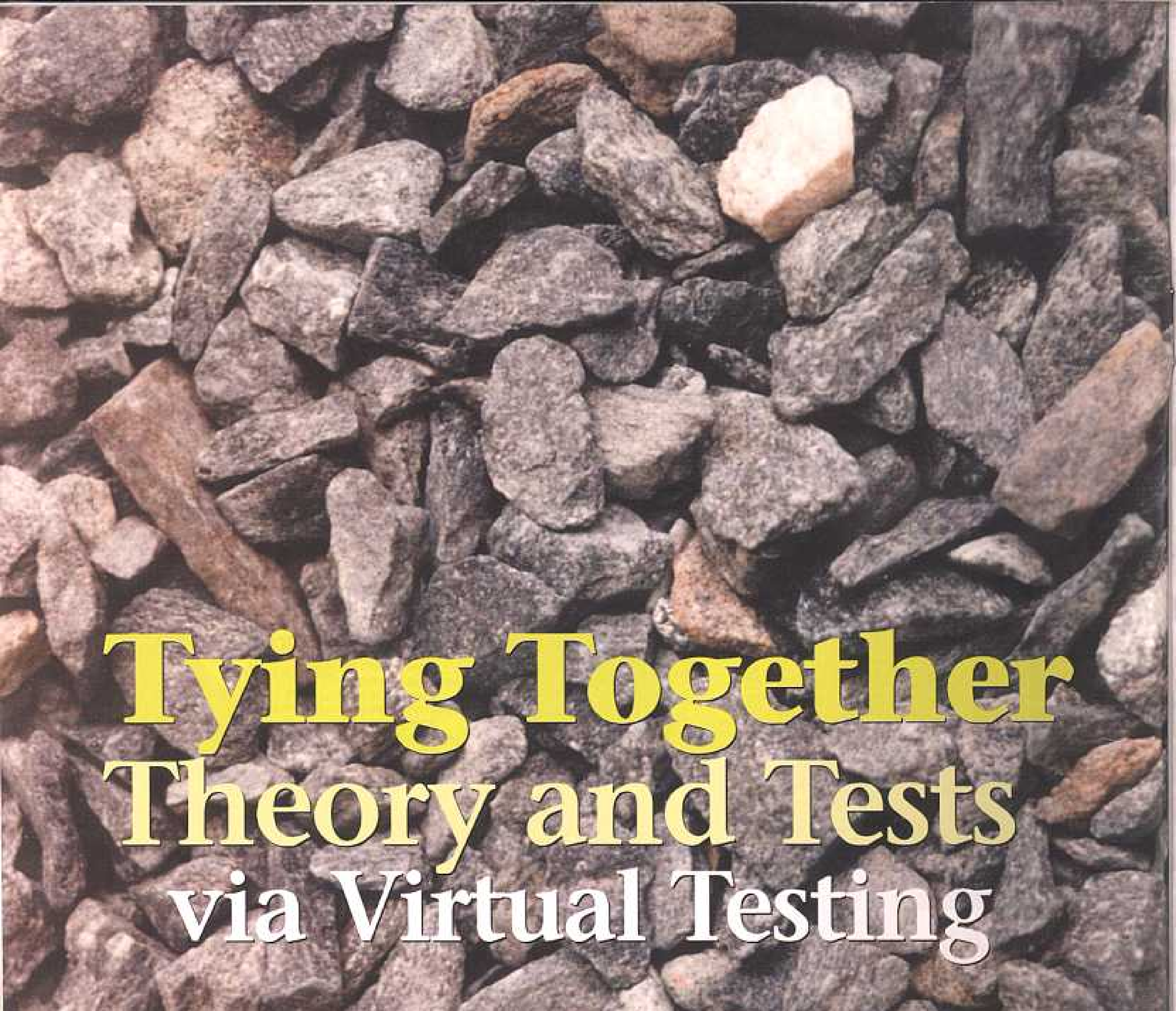

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by Edward J. Garboczi
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Do you ever dream about having an accurate idea of how aggregates from a new source will affect concrete pumpability without conducting countless slump tests (and slump tests may not give you the right answer, anyway)? Or, do you ever imagine figuring out how to make aggregates, which in the past have been considered sub-par because of alkali-silica reactivity problems, make money for you in a concrete-making application?

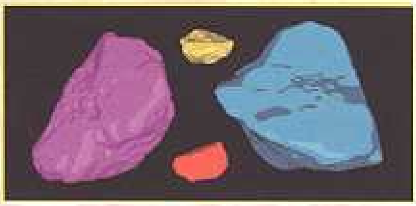
Do you ever wonder just how your microfine aggregates would affect concrete properties? And wouldn't it be nice if, after encountering seemingly odd results from a series of aggregate tests, you could explain these findings quantitatively and so understand and make use of these formerly puzzling results?

These kinds of scenarios are fulfilled all the time in the pharmaceutical, metal and semiconductor industries, because quantitative theory based on fundamental materials science has been successfully applied to these materials. Since the time of Sir Isaac Newton, the greatest advances in science have almost always involved the close cooperation of experiment and theory, and these materials are no exception to this rule.

Unfortunately, testing in the construction materials area has not had much quantitative theory to help guide and interpret it because construction materials like aggregates, portland cement concrete and asphaltic concrete are much too complicated for straightforward application of basic materials science. For example, the mathematical problem of packing random-shaped particles is still a very hard, unsolved problem. Fortunately, a new branch of materials science has arisen in the last 30 years. Called computational materials science, it has allowed direct application of the power of materials science to complicated materials like construction materials via the functionality of modern computers. The development of computational materials science has been directly linked to the modern revolution in information technology.

The leading computational materials science tool in the U.S. today for concrete is the Virtual Cement and Concrete Testing Laboratory (VCCTL), which is being developed at the U.S. National Institute of Standards and Technology (NIST) with the active cooperation of 10 leading corporations and associations in the concrete field: NSSGA, via the International Center for Aggregates Research (ICAR); Degussa Master Builders; Holcim (U.S.) Inc.; CEMEX; Sika Technology AG; W. R. Grace; Portland Cement Association (PCA); Association Technique de L'Industrie des Liants Hydrauliques (ATILH); Verein Deutscher Zementwerke eV (VDZ) and the National Ready Mixed Concrete Association. This large, integrated software package mimics a complete physical testing laboratory, with databases of cement and aggregates instead of bins and hoppers, material combination and concrete curing models instead of mixers and molds, a software interface instead of a cart to take materials and samples around the laboratory, and accurate models for performance prediction instead of instrumented testing machines.

Our idea is to be able to reduce the need for much routine testing, especially in the material development process, and make the remaining testing "smarter" by measuring fundamental material quantities that are needed by these kinds of models to be able to unleash their predictive power. An example of such a "sea-change" for a portland cement concrete test would be measuring fundamental rheological quantities with a rheometer instead of running empirical slump tests.



Some ways that the VCCTL could be used by industry include: (1) selecting a cement and some mineral admixtures, along with certain kinds of fine and coarse aggregates, and predicting concrete rheology (workability), (2) predicting what changes in a portland cement concrete or an asphaltic concrete will occur due to a shape change in aggregates, and (3) predicting the effect on concrete rheology due to the use of micro-fine aggregates of varying mineralogies.

To unlock the power of fundamental models, however, requires a higher level of material characterization than has heretofore routinely existed. The VCCTL aggregate database is a good example of this kind of information. In this database, we have not only various sizes of aggregates, but we have the actual 3-D shapes recorded mathematically. Using the information in this database, we can reconstruct actual aggregates from many different sources. The figure shown here is a montage of two fine and two coarse aggregates from different sources (we record actual shape, not actual color), displayed using Virtual Reality Modeling Language (VRML) technology adapted to normal Internet browsers. This combination of reality and model gives us an extraordinary ability to accurately predict real behavior for portland cement concrete and someday for other materials like asphaltic concrete.

In five years of cooperative work, we have progressed from version 1.0 to version 6.0 (to be released to the consortium early this year). The VCCTL is a challenging undertaking, because all its predictions are intentionally based on fundamental materials science and not empirical correlations. Only in that way can the VCCTL be flexible enough and accurate enough to accommodate changes in materials that come about for various reasons, *e.g.* changes in supply, changes in standards, or changes in location. Although some of the companies in the consortium are making effective economic use of the software already, in a few years we expect to have a version that is even more widely usable and practical. We also hope to develop and release, in 2006, an educational version of VCCTL that can be used by students across the country and the world to aid in their construction material training.

Sir Isaac Newton sparked the Industrial Revolution by inventing calculus to help him understand the physics problems he wanted to solve. As computational materials science-based models tie together testing and theory in the construction industry for the benefit of materials producers and selectors and users, what will be the result? The scenarios that were listed at the start of this article were only dreams—but some dreams do come true. ■