At its most basic, concrete is made from cement and aggregate, often Portland cement and gravel (or in Florida, limestone). Varying ingredients and their proportions directly influences the behavior of the final cement and concrete products. However, the full range of testing necessary to characterize the behavior of new concrete mixtures is an expensive and time-consuming task.

The chemistry of concrete is complex, but research has laid a foundation of knowledge about the chemistry of concrete's constituents that has allowed the National Institute of Standards and Technology to develop a software package, Virtual Concrete and Cement Testing Laboratory (VCCTL), that can predict the performance of concrete mixes. VCCTL requires an essential ingredient of its own to make accurate predictions: thorough characterization of the materials being simulated, especially in the case of materials drawn from a specific location, such as Florida limestone.

In this project, University of Florida researchers performed a systematic evaluation of materials used in Florida concrete mixtures and simulated them with VCCTL. In a two-phase program, researchers evaluated the effectiveness of VCCTL for prediction of concrete performance. First, techniques required to characterize Portland cement were developed and implemented, and the resulting virtual materials were simulated. Second, a testing program was performed on physical specimens to evaluate the accuracy of those simulations. The software's accuracy in predicting properties of concrete such as strength, elastic modulus, and time of set were examined.

VCCTL requires the chemical and physical properties for any materials included in the simulated concrete. Some additional inputs are not required but may improve the accuracy of the simulation. To obtain these inputs, researchers used various analytical techniques, including x-ray powder diffraction, laser particle-size analysis, scanning electron microscopy, and multispectral
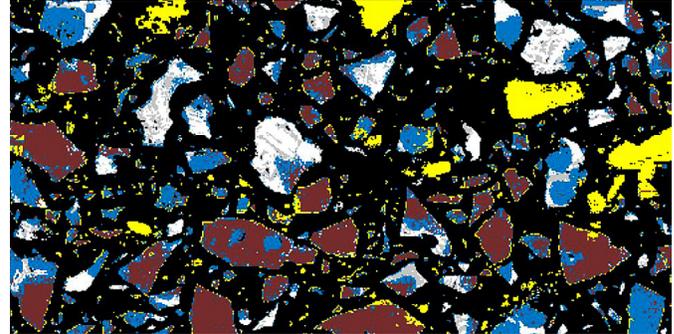
Multispectral analysis of concrete produces a false-color image. The colors represent different chemical phases within the concrete sample.

image analysis. Many standard test methods were used, such as the Blaine air-permeability test for cement fineness (ASTM C 204) and isothermal conduction calorimetry for heat of hydration (ASTM C 1702).

Seven concrete mixtures were simulated with VCCTL. All mixtures contained cement, water, fine aggregate, and coarse aggregate in varying proportions. VCCTL cannot yet model supplementary cementitious materials, so Portland cement was the only such material used. Three mixtures contained an admixture, either a Type D or a Type F (at two dosages). Water-to-cement ratio varied from 0.4 to 0.55. Each mix was also prepared as a physical sample according to ASTM C 192. Physical specimens were tested for slump, unit weight, temperature, air content, compressive strength, elastic modulus, time of set, and heat of hydration. Isothermal calorimetry was performed on physical mixes containing admixtures. A detailed comparison was made of simulated measurements to physical measurements of concrete properties.

Improving the accuracy of chemical simulation programs has led to advances in materials in many areas of engineering and the sciences. Projects like this one advance the capabilities of concrete simulations with the possibilities of developing new and more effective concrete mixes.