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The first of a two-part series on the materials science of fine particles. Guest Editor Egon Matijević, Distinguished University Professor, Department of Chemistry, Clarkson University.

POSTERMINARIES

By Any Other Name

Have you noticed a dual terminology when describing nonexperimental science? Do you have a theory or model to explain the difference between theories and models? Have you also observed that greater prestige seems to accrue to theories, and likewise to theorist as opposed to modeler? Why...? Perhaps models suffer from sounding like toys or mere imitations of reality.

As a student, I was taught theories. These were explanations usually expressible in mathematically closed form, at least under simplifying assumptions, and were derived from rather fundamental physical laws. The invoked combination of laws produced predictions tested by experiments which validated the theory within some limit of error. My sense was that if anything was called a model, there was an implied modifier such as "phenomenological," "heuristic," "*ad hoc*," or "empirical." From this, I presume that some or all of the relevant basic laws were unused or unknown and "seat-of-the-pants" guesswork helped produce an algorithm from which one could predict experimental results. Limits-of-error for a theory's validation combined experimental error with uncertainty in values of constants in the theory. For a model's validation, the additional, and *a priori* unquantifiable, incorrectness of the model enters as well. That is, you can't know how much of the mismatch to experiment is the model itself missing the mark. Theories do contain assumptions, and theoretical computation relies on approximations at some level. After what number, or degree of seriousness, of these deviations from absolute truth does a theory become a model?

Lately, the term modeling seems to arise much more often. In fact, some institutions will now seek to hire modelers *per se*. My sense is that these modelers are supposed to be a more practical breed and will not spend time with their heads in the clouds of theory for theory's sake. With the advent of more and better supercomputers, the numerical model calculation (often called simulation) has become more prevalent (i.e., more viable for a wider range of problems). Of course, these machines must also enable more complex computations of the theoretical variety. Somehow, numerical simulation lacks the elegance of closed analytical forms in both cases. Perhaps one distinction to be made is between the lengthy iterative self-consistent computations of theory and the theory-based lengthy statistical simulations, such as Monte Carlo, which extend theory to large-number systems.

There's another distinction in viewpoint to reckon with. One person's theory is another's model. Or perhaps one should say a "macroperson's" theory is a "microperson's" model. For example, if plotting the logarithm of your atomic diffusion data against inverse temperature yields a straight line, one can safely assume that an activated process is involved. The exponential behavior and the 1/T exponent are on firm theoretical ground, but the constant in the exponent, i.e., the activation energy, becomes a phenomenological parameter inaccessible to macroscopic computational approaches. There are many approaches to the calculation of microscopic properties, all deriving from accepted theory (i.e., Hamiltonians, wave equations, etc.), each choosing different ways to segment the problem with different assumptions and approximations. These may compute our activation energy and be regarded from the micro viewpoint as a theory, but it will be based on a "model" of what is important for the calculation.

How much of the distinction between theory and model is substantive and how much is semantic is not at all clear. And it is probably not an urgent question provided both contribute to our understanding of physical phenomena and our ability to predict the behavior of physical systems without creating an elitism-based stratification of the research community.

E.N. KAUFMANN

Expanding the Horizons of Our Terminology

The scale or index by which one can measure (or at least discuss) the degree to which a proposed theory deviates from tradition is called "exoticity."

A lack of homogeneity too fine to be called inclusions, second phases, spinodal decomposition, etc., and yet extending over several unit cells of the lattice is termed "mesoscopic" inhomogeneity. (This may imply the same scale as does the term "microcrystalline" which has been used to equivocate about not-quite amorphous solids.)

From a seminar, "Comments on the Theory of High Temperature Superconductivity," Morrel Cohen, (Exxon) presented at Argonne National Laboratory, July 27, 1989.