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Visualization in Classical Thermodynamics

A Difficult Subject Made Manageable Through Visual Thinking

"The time is upon us to use artistic methods and our magnificent modern graphics tools to show scientific ideas visually and to have pictures become the equal of numbers in dialogue among educated people."

The macroscopic thermodynamics of equilibrium ("classical thermodynamics") is often poorly understood. Students dislike the subject, most faculty dislike teaching it, and the net gain from much of entry-level instruction is discouragingly small. Modern thermodynamic analysis was laid out 140 years ago by Josiah Willard Gibbs, an unknown professor of mathematical physics at Yale University. Earlier, Gibbs had received this country's first Ph.D. in engineering after writing a dissertation on the subject of gears.

As studied today, thermodynamics is based on four unprovable -- but never disproven -- Laws. Professor Peter Atkins, the well-known Oxford author of chemistry textbooks, calls them: ***Four Laws That Drive the Universe***. Following the Laws logically leads to an array of state or "potential" functions that describe the behavior of systems interacting at equilibrium with their environments to produce or consume heat and work. A crucial part of that description is the specification of **limits** to these transfers of energy.

Gibbs wrote three seminal papers. The second paper was entitled: **A Method of Geometrical Representation of the Thermodynamic Properties of Substances by Means of Surfaces**. In it he used a **visual analogy** to explain how the spatial geometry of one particular state function (energy-entropy-volume) yields common physico-chemical properties such as pressure, temperature, volume, and the like. In this regard, Gibbs was an early, **if not the first**, scientific visualizer in this country.

The display assembled here shows the results of a career-long effort to use computer graphics to show the geometrical-mathematical-physical-chemical connections that Gibbs wrote about. Others have attempted this in the past, using manual methods to create plane diagrams, sculptures, even stereo drawings -- beautiful objects of art. But thermodynamic analysis is too complex, the mathematics too demanding, and the geometries involved too delicate for hand labor. **It is a job only for the computer.**

Listed above are the bright, motivated students who have made these creations possible. Without them, without the support acknowledged at the bottom, and without the encouragement of a small number of intellectually sensitive colleagues at Iowa State and other universities, there would be no results -- only vague promises.

There are two broad categories in this display:

I Parametric, three-dimensional models of thermodynamic potential functions in the various transformed coordinate systems used commonly for analysis.

The Gibbs Models — See the Web site, the examples shown in the Power Point presentation, and our recent paper, **"Visualizing the Gibbs Models"** (*Industrial and Engineering Chemistry Research*). See also the background information on the 2005 U.S. postage stamp honoring J. W. Gibbs (design contribution by K. R. Jolls).

II Tutorial software for producing surface and line drawings of phase diagrams – the unique set of derivative functions (equations of state) that involve measurable variables only.

"Equations of State" EOS — An early, technically outdated, but pedagogically successful attempt to use basic line graphics to show **thermodynamic processes** occurring on the surface of a PVT phase diagram. Fixed and moving displays are possible. EOS was used by many engineering departments in the late 1980s.

"ThermoGraphics" — Movable images of **fixed data sets** for thermodynamic vapor-liquid equilibrium (VLE: two- and three-component, fluid-phase mixtures). Developed on a Silicon Graphics computer using the "Showcase" utility – ported later to Windows for distribution.

"Animate" — Movable images derived from **multiple fixed data sets** for three- and four-component VLE systems. "**Animate**" shows the full functional content of thermodynamic VLE data that occupy more than three dimensions.

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