Advantages of 'Variational' Thermodynamics

Bob Eisenberg

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Written for Craig Evans

1) Variational thermodynamics puts spatial variables into theoretical chemistry, while connecting to the classical free energy formulations of the last 130 years. The free energies of classical chemistry become part of the 'energy' terms of the variational approach.
2) Boundary conditions appear inevitably and naturally.
3) Thus devices appear naturally and comfortably. For example, variational themodynamics can describe systems with inputs and outputs, An ordinary voltage amplifier has an homogeneous Neumann condition as the input and an inhomogeneous Dirichlet as the output, with the value of the inhomogeneity determined by (and often proportional to) the voltage (function value) at the input.
4) Flow and nonequilibrium properties appear as the inevitable consequence of the classical chemical free energies and boundary conditions. In chemical language, the variational approach allows one to have two different concentrations, whereas classical thermodynamics allows only one spatially uniform concentrations.
5) Components can be added consistently. Most experimental science changes systems and examines the result. A very common strategy is to add a component to the system. If a component is added in the variational approach, the resulting differential equations are always consistent (as long as the algebra is correct) and the number of adjustable parameters is minimal.
6) All of life and much of chemistry (nearly all of chemistry before say 1960) occurs in ionic solutions. Ionic solutions contain charges that are coupled each to everyone by the electric field. Ionic solutions are most important in devices and biology where they are concentrated. Steric interactions are of great importance in concentrated solutions. Two ions cannot occupy the same space. Variational thermodynamics handles interacting systems naturally and consistently.
7) Chemical reactions (involving changes in electron distributions) occur very very quickly (e.g., 10^{-18} sec). Chemical reactions are very sensitive to local concentrations (number density). Number density fluctuates dramatically on time scales very long indeed compared to 10^{-18} sec. Flutuations occur from say 10^{-9} sec onwards (i.e., faster). Thus, chemical reactions are likely to occur in small spatial inhomogeneities in concentration with properties (e.g., concentrations) very different from averages over space (and time). Classical chemistry ***only*** uses averages over space and time in trying to explain chemical reactions. Variational thermodynamics can help replace the

classical approach, as multiscale stochastics are woven into the existing tapestry of variational thermodynamics