The Maintenance of a Lifelong Bibliographic Database

—

with Emphasis on Thermodynamics Applied to Phase & Reaction Equilibria and Continuum Physics; and the Mathematical Description, Computer Programming and Calculation of Property Changes and Physical Conditions in said Systems

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Foreword

This database has matured over three decades of research related to all kinds of problems related to thermodynamics, and especially to the mathematical description of thermodynamic equilibrium problems. No attempt has been made to create a complete database for any of the projects, but as it stands the database has a number of links to older literature and lesser-known assets, which may prove valuable to the next generation of researchers. Among several industrial projects and academic research topics covered by the database, I would like to mention:

(1) Experimental data
  (a) $NaF - AlF_3 - Na_3AlF_3$
  (b) $HCl - H_2O$
  (c) $HNO_3 - H_2O$
  (d) $HCOOH - H_2O$
(2) State description
  (a) Equations of state
  (b) Excess energy models
  (c) Electrolyte theory
  (d) Continuous thermodynamics
  (e) Thermodynamic shocks
(3) Thermodynamic theory
  (a) Phase equilibrium
  (b) Phase stability
  (c) Critical points
  (d) Chemical equilibrium
(4) Applications
  (a) Exergy analysis
  (b) Finite time thermodynamics
  (c) Irreversible thermodynamics
  (d) Differential scanning calorimetry

About two-thirds of the articles referenced in the database, and a good number of the books, are available as scanned documents or downloaded PDF files. These files cannot (currently) be released for public use without violating copyright, but most universities are equipped with good online services, so this should not cause a serious problem for academic research staff.

CHAPTER 1

Cross-sectional Topics

My Private Library (thwlib)

All kinds of books and articles dealing with mechanics, technical hobbies and the history of technology and science. However, a good part of the literature is hard science, including thermodynamics, physics, mathematics and chemistry.

Related keywords: thwlib.

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Biographies (biography)

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Related keywords: biography.

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Historical Notes (histor(y,ical))

Books and articles of historical interest, also including a few biographies and discussions of the impact of science (and named scientists) on modern society.

Related keywords: history | historical.

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Miscellaneous (Misc)

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CHAPTER 2

Phase and Matter

Binodal Curves (PhMatB)

The calculation of phase boundary curves, and not to mention the complete modelling of assessed phase diagrams, covers a vast literature. In most cases, they are purpose-built numerical procedures that require clever initializations and a lot of heuristics. The ultimate difficulty, however, occurs when the phase boundary has one, or at worst several, critical endpoints.

Related keywords: phase & boundary | binodal & curve | phase & diagram | saturation.

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Criticality (PhMatC)

Direct calculation of critical points.

Related keywords: critical | tricritical.

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Metastability (PhMatM)

Metastability in general and the limiting negative pressure of fluids in particular.

Related keywords: metastable | spinodal | negative & pressure | superheating.

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Phase Equilibrium (PhMatP)

Phase equilibrium calculation. Most of the literature is about 2-phase VLE and 3-phase VLLE formulations since these are important for the oil and gas industry, but there are also a good number of general algorithms.

Related keywords: (multicomponent | multiphase) & equilibrium.

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Chemical Equilibrium (PhMatR)

Chemical equilibrium in homogeneous (gas) phases and combined chemical and phase equilibrium calculations. Most of the literature is about the homogeneous (ideal) gas case, but there are also a good number of articles about VSE formulations. Unfortunately, there are few articles on the general formulation of the problem.

Related keywords: simultaneous | (& phase & reaction) & equilibrium.

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Global (intrinsic) Stability (PhMatS)

Methods for the global minimization of equilibrium problems, typically using the Gibbs' tangent plane criterion.

Related keywords: stability | global & minimum | uniqueness | tangent & plane | phase & split.

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Transport Phenomena (PhMatT)

Methods and data for (mostly) diffusion theory.

Related keywords: transport & phenomena | diffusion | maxwell & stefan.

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CHAPTER 3

Thermodynamics

Computer Algebra Systems (TheCAS)

The borderland between thermodynamics, computer programming and thermodynamics databases.

Related keywords: thermodynamics & (computer & algebra | software | object & oriented | database).

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Differential Scanning Calorimetry (TheDSC)

Calorimetry in general and Differential Scanning Calorimetry in particular.

Related keywords: differential & scanning & calorimetry | dsc.

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Extended Thermodynamics (TheExt)

Thermodynamics of systems that are subject to external fields and to capillary forces etc.

Related keywords: extended & thermodynamics | gravity | gravitational | electromagnetic | surface & energy.

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Classical Thermodynamics (TheCla)

The description of simple systems in T, p, N and T, V, N coordinates. Gibbsian thermodynamics mostly. There are also some articles and the not-so-simple description in generalized coordinates.

Related keywords: thermodynamics | classical | (simple & systems) | gibbsian.

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Continuous Thermodynamics (TheCon)

Non-discrete description of polydisperse systems, polymers, hydrocarbon fluids, etc.

Related keywords: thermodynamics & continuous.

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Finite Time Thermodynamics (TheFin)

Finite time thermodynamics. Analyses of machinery.

Related keywords: thermodynamics & (finite & time | optimum & work | machines).

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Irreversible Thermodynamics (TheIrr)

Onsager irreversible thermodynamics and transport phenomena (not radiation).

Related keywords: thermodynamics & irreversible | transport | diffusion.

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Second Law Analyses (The2nd)

Second law analysis of chemical plants, energy availability studies, exergy efficiency, etc.

Related keywords: second & law | exergy & analysis.

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CHAPTER 4

Thermodynamic Models

Semi-Empirical Correlations (ModCor)

Semi-empirical models other than thermodynamic ones, general correlations, corresponding state principle, etc.

Related keywords: empirical | correlations | corresponding & state.

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Electrolyte Models (ModEle)

Excess Gibbs energy models for electrolytes.

Related keywords: (activity & coefficients | excess & gibbs & energy | thermodynamic & properties) & electrolytes & (aqueous | mixed & solvent).

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Equations of State (ModEOS)

Equation of state models in Helmholtz (fluids mostly) and Gibbs energy (solids mostly) representations, i.e. $p = p(T, V, N)$ and $V = V(T, p, N)$.

Related keywords: pvt | eos | fundamental & (helmholtz & energy | gibbs & energy) | equation & of & state | surface.

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Parameter Regression (ModFit)

Parameter regression of physical models.

Related keywords: parameter & (fitting | estimation | regression) | maximum & likelihood | least & squares.

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Gas hydrates and clathrates (ModHyd)

Thermodynamic models for gas hydrates or so-called gas clathrates. Most of the models are derived from Van der Waals – Platteuw theory.

Related keywords: gas & hydrate | clathrate.

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Lattice Structure Models (ModLat)

Excess Gibbs energy models for electrolytes (mainly), metallic, and intermetallic systems.

Related keywords: sublattice | quasichemical | cell & theory | lattice & structure | metallic & alloys | temkin.

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Models for Molecular Fluids (ModMol)

Excess Gibbs energy models for non-electrolytes.

Related keywords: (nonpolar | molecular) & excess & gibbs & energy.

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CHAPTER 5

Applied Sciences

International Union of Pure and Applied Chemistry (IUPAC)

Operative definitions and standards in chemistry and thermodynamics.

Related keywords: iupac | terminology | definitions | conventions.

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Physics (Phys)

Classical physics, fluid mechanics, relativity, quantum mechanics, etc.

Related keywords: physics | (continuum | fluid) mechanics & radiation | field & theory.

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Chemistry (Chem)

Inorganic, organic, and physical chemistry.

Related keywords: chemistry.

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Chemical Engineering (ChemEng)

Traditional chemical engineering displines: two-film theory, distillation, heat exchangers, membranes, etc.

Related keywords: chemical & engineering | unit & operations | twofilm (very spefic).

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Metallurgy & metallic materials (Metal)

Extractive and physical metallurgy, iron and steels and metal based materials.

Related keywords: metals | metallurgy.

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Computer Programming (Prog)

Programming languages and issues, and tools for dealing with such things.

Related keywords: programming | paradigms | software | implementation | algorithm | computer & language.

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Mathematics (Math)

Applied and engineering mathematics, optimization, algebra, calculus, etc.

Related keywords: mathematics.

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Optimization (OptMet)

Theory and applications of optimization, and (non)linear programming.

Related keywords: optimization.

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Linear Algebra (LinAlg)

Numerical linear algebra and numerical tensor & vector calculus.

Related keywords: linear & algebra | matrix | tensor | vector & space.

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CHAPTER 6

Numerical Calculations

Numerical Methods (NumMet)

Applied & Engineering numerical methods.

Related keywords: numerical & (method | mathematics | algorithm).

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Calculating Phase Diagrams (CALPHAD)

So-called CALPHAD assessments.

Related keywords: (assessed | assessment) & (phase & diagrams) & (solid | liquid| vapor | vapour) | (metal | ceramic | salt).

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Flowsheet calculations (Flowsheet)

Chemical process calculations.

Related keywords: flowsheets | networks | solvers | chemical & processes.

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Automatic Differentiation (Diff)

Automatic (computerized) differentiation.

Related keywords: automatic & differentiation.

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CHAPTER 7

Experimental Data

Standard State Properties (DatPCD)

Standard state properties for pure components.

Related keywords: barin | janaf | dippr | etc.

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Mineral Acids (DatAci)

Experimental data for aqueous solutions of HCl, H_2SO_4, HNO_3, etc.

Related keywords: (experimental | data) & acids.

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Nitric acid (hno3)

Papers related to the thermophysical properties of pure HNO_3 and its aqueous solutions (nitric acid). Including thermodynamic models and other theoretical aspects as well as experimental data. Beyond also the simple binary $HNO_3 - H_2O$.

Related keywords: no2 | n2o4 | n2o5 | hno2 | nitric\ acid | (nitrogen | nitrous | nitric)\ (per)?oxide(s)?

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Formaldehyde (DatCHOH)

Experimental data for formaldehyde.

Related keywords: (experimental | data) & hcoh | (ch3coh & h2o).

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Cryolite (DatCry)

Experimental data for $NaF-AlF_3-Al_2O_3$ plus CaF_2, LiF, etc.

Related keywords: (experimental | data) & cryolite | naf | alf3 | na3alf6 | al2o3.

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Electrolytes (DatEle)

Experimental data for aqueous salt solutions and electrolytes in general.

Related keywords: (experimental | data) & electrolytes | aqueous & solutions.

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Gases and Fluids (DatGas)

Experimental p, V, T and thermal data for gases and dense fluids.

Related keywords: (experimental | data) & (gases | dense & fluids) | pvt | enthalpy | heat & capacity.

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Water and Heavy Water (DatH2O)

Experimental data for water and heavy water.

Related keywords: (experimental | data) & (water | h2o | heavy | d2o).

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Hydrocarbons (DatHyC)

Experimental data for alkanes, alkenes, alkynes, aromates, etc.

Related keywords: (experimental | data) & hydrocarbons.

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Liquids (DatLiq)

Experimental data for liquids (different from gases and fluids).

Related keywords: (experimental | data) & liquids.

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Minerals (DatMin)

Experimental data for (clay) minerals.

Related keywords: (experimental | data) & minerals.

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Ammonia (DatNH3)

Experimental data for ammonia, water, nitrogen and hydrogen needed for ammonia synthesis calculations.

Related keywords: (experimental | data) & (ammonia | nh3).

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Molten Salts (DatSal)

Experimental data for simple molten salts of sodium, potassium, ammonium, etc.

Related keywords: (experimental | data) & (salt | melts).

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Solids (DatSol)

Experimental p, V, T data of pure solid phases.

Related keywords: (experimental | data) & solids.

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Urea (DatUrea)

Experimental data for urea, biuret, CO_2 and water at urea synthesis conditions.

Related keywords: (experimental | data) & urea | biuret.

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