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Equations of State and Fluid Dynamics

(Lecture Notes)

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1. Thermodynamics: basics

- Thermodynamic variables
  Fundamental
  Derived
- Fundamental identity
  Thermodynamic laws
  Phase space
  Implicit assumption
- Key EOS parameters
  Dimensionless parameters
- Consistent units
  Fundamental units
  Standard unit systems
- Exercises
  1.1 Example of key parameters
  1.2 Dimensional analysis

2. Fluid equations (1-D)

- Conservation form
- Euler equations
  Entropy equation
- Characteristic form
  Relaxation phenomena
  Rarefaction wave
- Incomplete EOS
  $P(V, e)$ EOS
  $P(V, T)$ EOS
  Extend to complete EOS
- Exercises
  2.1 Expression for sound speed
  2.2 Crossing of characteristics
  2.3 Escape velocity

3. Thermodynamics: advanced

- Thermodynamic potentials
  Thermodynamic stability
  Legendre transform
  Standard potentials
- Thermodynamic identities
- Phase transition
  Phase portrait
  Equilibrium EOS
- Exercises
  3.1 Grüneisen coefficient
  3.2 Isentropic & isothermal bulk moduli

4. Thermo-Elastic solid

- Elastic models
- Stress & Strain tensors
  Model free energy
  Elastic flow equations
- Moduli
- Acoustic waves
- 1-D uniaxial strain
- Phase transtitions
- Exercises
  4.1 Acoustic wave speeds

5. Hugoniot locus

- Jump conditions
  Hugoniot equation
  Weak shock
- Riemann problem
  Graphical solution
  Examples
  EOS constraints
- Shock change equation
- Numerical algorithms
  Front tracking
  Shock capturing
- Exercises
  5.1 Ideal gas shock locus
  5.2 Linearized Riemann problem

6. Shock stability

- 1-D stability
  Characteristic criterion
- 2-D stability
  Analyses of D'yakov and Erpenbeck
  Analyses of Kontorovich and Fowles
- Digression
  Shock polars
  Whitham-Chisnell shock dynamics
- Exercises
  6.1 Weak shocks
  6.2 Oblique shocks

7. Hugoniot locus for phase transition

- Equilibrium wave structure
  (V, P)–plane
  (u_p, u_s)–plane
  (u, P)–plane
- Rate dependent effects
  Elastic-plastic transition
  Wave structure
  Example
- Exercises
  7.1 Triple shock rule

8. Measurement of shock locus

- Example data
  Illustrative Hugoniot loci
- Methods to generate shocks
- Calibrate standard
  Principal Hugoniot locus
  EOS off principal locus
- Impedance match experiments
  Measure sample
- Exercises
  8.1 Shock pressure from plate impact
  8.2 Explosive driven flyer

9. Experimental isotherm & isentrope

- High pressure experiments
  Isotherm
  Isentrope
- Case study
  HMX isotherm
- Exercises
  9.1 Ordering of loci

10. Mie-Grüneisen EOS

- Incomplete EOS
  Fitting form
  Reference curve
  Grüneisen coefficient
- Complete EOS
  Grüneisen coefficient
  Temperature
- Common solid EOS
  Linear u_p-u_s Hugoniot relation
  Domain of model EOS
- Shock polar
- Exercises
  10.1 Sound speed
  10.2 Linear u_p-u_s Hugoniot

11. Debye model

- Helmholtz free energy
  Decomposition
  Phonon contribution
- Debye approximation (acoustic modes)
  Density of states
  Phonon free energy
  Mie-Grüneisen EOS
  Specific heat
- Optical modes
  Free energy
  EOS
- Exercises
  11.1 Temperature scale

12. Statistical mechanics

- Configuration space
- Statistical ensembles
  Microcanonical ensemble
  Canonical ensemble
  N–P–T ensemble
- Atomic potentials
  Born-Oppenheimer approximation
  Quantum chemistry
- Computational techniques
  Molecular dynamics
  Monte Carlo
- Numerical experiments
  Thermodynamic quantities
  Uncertainties in simulated results
- Exercises
  12.1 Free energy

13. Simple analytic EOS

- Perfect gas
  Free energy
  Domain
  Generalization
- Stiffened gas
  Free energy
  Domain
- Hayes EOS
  Free energy
  Complete EOS
  Domain
  Example
- Exercises
  13.1 Thermally perfect gas
  13.2 Van der Waal EOS

14. Generalized Hayes EOS

- Hayes EOS
  Free energy
- Thermal component
  Grüneisen coefficient
  Specific heat
- Reference isotherm
  Birch-Murnaghan EOS
  Vinet EOS
  Empiricism & validation
- Exercises
  14.1 Grüneisen coefficient
  14.2 Hayes EOS reference energy
  14.3 Hugoniot locus

15. Semi-analytic EOS

- Porous materials
  - Free energy
  - Equilibrium model
  - Hugoniot loci
- P-T equilibrium mixture
  - Free energy
  - Uniqueness & existence
  - Domain issue
  - Sound speed
- Chemical equilibrium
  - Free energy
  - Equilibrium model
- Two-phase EOS
  - Coexistence curve
  - Free energy
- Exercises
  - 15.1 P-T equilibrium