

MIT Course X PhD Qualifying Exam Study Guide

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Chapter 1

Multiscale Analysis

1.1 Basic Physics (1-1)

Physics (Box 1-1)

Descriptions of Matter, Energy, and Moments

Macro- and Micro- Views

Types of work interactions

$$\delta W = F \cdot d\underline{x}$$

Type of work	$F \cdot d\underline{x}$
Pressure-Volume	$-P \cdot dV$
Frictional	$F_f \cdot d\underline{x}$
Surface Deformation	$\sigma \cdot d\underline{a}$
Electrical Charge Transport	$\epsilon \cdot dq$
Electric Polarization	$E \cdot d\underline{D}$
Magnetic Polarization	$H \cdot d\underline{B}$
Stress-Strain	$\underline{V}_0(F_x/\underline{a})d\Omega = \underline{V}_0(F_x/\underline{a})dx/x_0$

1.2 Quantum

1.3 Single Molecule (7-2 – 7-4)

Potential Fundamentals (Box 7-2)

$$F = \frac{du}{dr}$$

$$\text{Coulombic interaction: } u \sim \frac{q_i q_j}{r}$$

$$\text{Dipole-Dipole: } u_{d-d} \sim \frac{-\epsilon_{dipole}}{r^6 kT}$$

$$\text{Dispersion-Attraction: } u_{att} \sim \frac{-\epsilon_{att}}{r^6}$$

$$\text{Repulsion: } u_{rep} \sim \frac{-\epsilon_{rep}}{r^{12}}$$

Mixing for Potential Functions (Box 7-3)

$$\sigma_{ij} = \frac{\sigma_{ii} + \sigma_{jj}}{2}$$

$$\epsilon_{ij} = \left(\epsilon_{ii} \epsilon_{jj} \right)^{1/2}$$

Potential (Box 7-4)

Ideal

- $\Phi(r) = 0$
- Parameters: none

Hard Sphere

- $\Phi(r) = \begin{cases} \infty & r \leq \sigma \\ 0 & r > \sigma \end{cases}$
- Parameters: σ

Square well

- $\Phi(r) = \begin{cases} \infty & r \leq \sigma \\ -\epsilon & \sigma < r \leq R\sigma \\ 0 & r > R\sigma \end{cases}$
- Parameters: σ, ϵ, R

Lennard-Jones

- $\Phi(r) = 4\epsilon \left[\left(\frac{\sigma}{r} \right)^{12} - \left(\frac{\sigma}{r} \right)^6 \right]$
- Parameters: σ, ϵ

Kihara

- $\Phi(r) = 4\epsilon \left[\left(\frac{\sigma - 2a}{r - 2a} \right)^{12} - \left(\frac{\sigma - 2a}{r - 2a} \right)^6 \right]$
- Parameters: σ, ϵ, a

Sutherland (ν dW)

- $\Phi(r) = \begin{cases} \infty & r \leq \sigma \\ -\epsilon \left(\frac{\sigma}{r} \right)^6 & r > \sigma \end{cases}$
- Parameters: σ, ϵ

1.4 Molecular Ensemble (2-1)

Statistical Mechanics (Box 2-1)

Goal: Connect quantum state of matter (microscopic) to classical thermodynamics (macroscopic).

Postulates

- Ergodic
 - Time averaging equivalent to ensemble averaging
- Equal A Priori Probabilities
 - States with equal $N, \underline{V}, \underline{E}$ are equally likely

$$\beta = \frac{1}{kT}, \quad \langle B \rangle = \sum P_i B_i, \quad \ln N! \approx N \ln N - N, \quad P_i = \frac{\exp(-\beta \underline{E}_i)}{\sum \exp(-\beta \underline{E}_i)}$$

1.5 Continuum

1.6 Macroscopic Analysis

Chapter 2

Thermodynamics

2.1 Statistical Mechanics and Calculus

2.1.1 Ensembles and Averaging (2-2 - 2-5, 3-1)

Microcanonical (Box 2-2)

Constant: $N, \underline{V}, \underline{E}$

Constraint Equations: $\sum n_i = \tilde{N}$

Partition Function:

$$\Omega \equiv \omega(\underline{E})$$

Natural Function: $S = k \ln \Omega$

Canonical (Box 2-3)

Constant: N, \underline{V}, T

Constraint Equations: $\sum n_i = \tilde{N}$, $\sum n_i \underline{E}_i = \underline{E}^{total}$

Partition Function:

$$Q_N \equiv \sum_{\underline{E}_i} \Omega \exp(-\beta \underline{E}_i) = \sum_{\underline{E}_i} \omega(\underline{E}_i) \exp(-\beta \underline{E}_i)$$

$$Q_N \equiv \sum_i \exp(-\beta \underline{E}_i)$$

Natural Function: $A = -kT \ln Q_N$

Grand Canonical (Box 2-4)

Constant: μ, \underline{V}, T

Constraint Equations: $\sum n_i = \tilde{N}$, $\sum n_i \underline{E}_i = \underline{E}^{total}$, $\sum n_i N = N^{total}$

Partition Function:

$$\Xi \equiv \sum_N \sum_{\underline{E}_i} Q_N \exp(\beta \mu N) = \sum_N \sum_{\underline{E}_i} \omega(\underline{E}_i) \exp(-\beta \underline{E}_i) \exp(\beta \mu N)$$

$$\Xi \equiv \sum_N \sum_i \exp(-\beta \underline{E}_i) \exp(\beta \mu N)$$

Natural Function: $P\underline{V} = kT \ln \Xi$

Isobaric/Isothermal (Box 2-5)

Constant: N, P, T

Constraint Equations: $\sum n_i = \tilde{N}$, $\sum n_i \underline{E}_i = \underline{E}^{total}$, $\sum n_i \underline{V}_i = \underline{V}^{total}$

Partition Function:

$$\Delta \equiv \sum_{\underline{V}} \sum_{\underline{E}_i} Q_N \exp(-\beta P \underline{V}) = \sum_{\underline{V}} \sum_{\underline{E}_i} \omega(\underline{E}_i) \exp(-\beta \underline{E}_i) \exp(-\beta P \underline{V})$$

$$\Delta \equiv \sum_{\underline{V}} \sum_i \exp(-\beta \underline{E}_i) \exp(-\beta P \underline{V})$$

Natural Function: $\underline{G} = -kT \ln \Delta$

2.1.2 Applied Statistical Mechanics (4-1 - 6-2)

Classical Approach (Box 6-1)

Criteria: $\Delta E/kT \ll 1$

$$Q_{cl} = Q_{int} Q_{cm} = Q_{int} Q_{trans} Z = \frac{Z Q_{int}}{\Lambda^{3N} N!}, \text{ classical partition coefficient}$$

- $\Lambda \equiv \left(\frac{h^2}{2\pi m kT} \right)^{1/2}$, thermal DeBroglie wavelength
- $Q_{int} = \frac{q_{int}^N}{N!}$, internal partition coefficient
 - o $q_{int} = q_{elec} q_{nuc} q_{vib} q_{rot}$, molecular partition coefficient
- $Z^* \equiv \int \dots \int \exp \left[-\frac{\Phi(\underline{r}^N)}{kT} \right] d\underline{r}^N$, configurational integral

Mean Field Theory (Box 6-2)

$$Z^* = \exp \left[-\frac{\langle \Phi(\underline{r}^N) \rangle}{2kT} \right]^N [\underline{V}_f]^N$$

$$- \langle \Phi(\underline{r}^N) \rangle = \frac{N \langle \rho \rangle}{2} \int_0^\infty \Phi_{ij}(r) g(r) 4\pi r^2 dr$$

- $g(r)$, radial distribution function
- $\Phi_{ij}(r)$, potential function

2.1.3 Property Frameworks

2.1.3.1 Fundamental Surface (13-1 - 13-6)

2.1.3.2 Legendre Transform (14-3)

2.1.3.3 EOS (7-1)

Virial (Box 7-1)

Form

- $p = \rho kT + kT \sum_{n=2}^{\infty} B_n(T) \rho^n = \rho kT(1 + B_2 \rho + \dots)$
- $B_2(T) = -2\pi N_A \int_0^{\infty} [\exp[-\beta \Phi(r)] - 1] r^2 dr$
 - Quantifies the two-body interaction
 - McMillan-Mayer TM 471
 - Hard sphere: $B_2 = \frac{2\pi\sigma^3}{3}$
 - Square well: $B_2 = \frac{2\pi\sigma}{3} \left[1 + (1 - \exp(\beta\epsilon))(R^3 - 1) \right]$
 - Lennard-Jones: $B_2(T) = -2\pi N_A \int_0^{\infty} \left[\exp \left[-\beta \left(4\epsilon \left[\left(\frac{\sigma}{r} \right)^{12} - \left(\frac{\sigma}{r} \right)^6 \right] \right) \right] - 1 \right] r^2 dr$

2.2 Property Relations

2.2.1 Models

2.2.1.1 Volumetric (14-2, 14-41)

2.2.1.1.1 Bridgeman (15-1 -18-1)

2.2.1.2 Non-Volumetric (23-1)

2.2.1.2.1 Energy Relationships (14-1)

2.2.2 Property Relations and Quantities

2.3 Mixture Properties (34-1)

2.3.1 Stability and Criteria (19-1 - 19-2)

2.3.2 Gibbs-Duhem (24-1)

2.3.3 Microscopic Mixing (8-1 - 9-3)

Osmotic Pressure (Box 8-1)

Vant Hoff Formulation (ideal)

- $\Pi = C_s RT$
- Parallel to Ideal Gas Law ($C_s = N/V$)

Equilibrium Approach

- $\mu_w(T, 1\text{bar} + \Pi, x_s) = \mu_w(T, 1\text{bar}, \text{pure}) + RT \ln \gamma_w x_w + \int_1^{1+\Pi} \bar{V}_w dP$
- For incompressible

$$\blacksquare \quad \ln(\gamma_w) \approx -\ln(x_w) - \frac{\Pi \bar{V}_w}{RT} \text{ with } x_w = 1 - x_s$$

Statistical Mechanics Approach

– McMillan-Mayer Theory

○ Grand Canonical Function as natural variable

$$\blacksquare \quad \ln(\Xi) = \frac{(P + \Pi)V}{kT}$$

○ Under dilute solution limit,

$$\blacksquare \quad \frac{\Pi}{kT} = \rho_2 + B_2 \rho_2^2 + \dots$$

$$\blacksquare \quad \frac{\Pi}{C} = \frac{RT}{M_W} + \frac{B_2 NRT}{(M_W)^2} C + \dots$$

• Graph of (Π/C) v. C

$$\circ \quad \text{Intercept: } M_W = \frac{RT}{(\Pi/C)_{C \rightarrow 0}}$$

○ Assuming Pairwise additivity

$$\blacksquare \quad B_2 = -2\pi \int_0^\infty \left(\exp \left[\frac{-\langle \Phi_{12} \rangle}{kT} \right] - 1 \right) r^2 dr$$

■ For Hard Sphere Interactions

$$\bullet \quad B_2 = \frac{16}{3} \pi b_0^3, \quad B_3 = \frac{5}{8} B_2^2$$

○ Using a ΔG^{EX} function

$$\blacksquare \quad -\bar{V}_1 \Pi = RT \ln a_1$$

• Flory-Huggins (11-66)

- $\frac{\partial \Delta G^{EX}}{\partial N_1} = RT \ln a_1$

Flory Huggins Theory (Box 8-2)

$$\Delta G_{mix} = RT[N\phi_1\phi_2\chi + (x_1 \ln \phi_1 + x_2 \ln \phi_2)]$$

$$\frac{\partial \Delta G_{mix}}{\partial x_1} = \mu_1, \quad \frac{\partial \Delta G_{mix}}{\partial x_2} = \mu_2$$

$$N_1 = V\phi_1 \text{ and } \phi_2 = \frac{nN_2}{N_1 + nN_2}$$

Binodal

$$- \quad \mu_1 - \mu_1^0 = RT \left[\ln(1 - \phi_2) + \left(1 - \frac{1}{n}\right) + \chi \phi_2^2 \right]$$

$$- \quad \mu_2 - \mu_2^0 = RT \left[\ln \phi_2 + (1 - \phi_2)(1 - n) + \chi(1 - \phi_2)^2 \right]$$

Spinodal

$$- \quad \frac{\partial^2 \Delta G_{mix}}{\partial x_2^2} = 0 = \frac{\partial \Delta \mu_1}{\partial \phi_2} = -\frac{1}{1 - \phi_2} + 1 - \frac{1}{n} + 2\chi \phi_2$$

Critical Point

$$- \quad \frac{\partial^3 \Delta G_{mix}}{\partial x_2^3} = 0 = \frac{\partial^2 \Delta \mu_1}{\partial \phi_2^2} = -\frac{1}{(1 - \phi_{c,2})^2} + 2\chi_c$$

$$- \quad \chi_c = \frac{1}{2\phi_{1,c}} + 1 - \frac{1}{n} + \frac{1 - \phi_{1,c}}{\phi_{1,c}^2} = 0$$

$$- \quad \chi_c = \frac{1}{2}(1 + n^{-1/2})^2$$

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a
 A
 B
 B
 B_i
 Bi
 Br
 c_D
 C
 C_P
 C_V
 D
 D_{ij}
 D_i
 Da
 D_e
 D_0
 \underline{e}_i
 \underline{e}
 E
 E
 \widehat{f}
 \widehat{f}
 $f_{\underline{e}_i}$
 F
 F_B
 $g(r)$
 G
 Gr
 h
 H
 \mathcal{H}
 H
 \mathcal{H}_i
 H_V
 i
 I
 J_i
 k
 $k_{c,i}$
 K
 K
 \mathcal{K}_i

K_a
 K_P
 K_y
 K_γ
 K_ϕ
 L
 m
 M_W
 \underline{n}
 N
 N_i
 Nu
 P
 P
 Pe
 Pr
 q_i
 q
 q_{elec}
 q_{int}
 q_{nuc}
 q_{rot}
 q_{trans}
 q_{vib}
 $q^{(x)}$
 Q
 Q_{int}
 Q_{cl}
 Q_{cm}
 Q_N
 r
 R_V
 Ra
 Re
 S
 S_A
 \underline{S}
 Sc
 Sh
 Sr
 t
 T
 u
 U
 U

v
 V
 V_f
 \underline{w}
 $\underline{\underline{w}}$
 W
 x
 x_i
 x_i
 z
 z_i
 Z
 Z^*
 α
 β
 β
 β_i
 γ_i
 γ
 $\underline{\underline{\Gamma}}$
 δ
 Δ
 $\epsilon_M, \epsilon_i, \epsilon_E$
 ϵ
 η
 η
 Θ
 Θ_ν
 Θ_n
 κ
 λ
 λ
 λ
 Λ
 μ
 μ
 ν
 ν
 ν_{ij}
 ν_i
 ξ
 ξ
 Ξ
 Π
 ρ

σ
 σ
 $\underline{\underline{\sigma}}$
 τ
 τ_{ij}
 ϕ_i
 ϕ
 ϕ
 Φ
 Φ
 $\Phi_{ij}(r)$
 Φ_n
 χ
 Ψ
 Ψ
 ω
 ω
 ω_e
 Ω
 Ω_{mix}
 \mathfrak{S}
 \wp
 \mathcal{R}
 c
 e
 g
 \mathcal{F}
 h
 $\backslash \text{av}$
 R
 k_B
 π
 x
 \underline{x}
 $\underline{\underline{x}}$
 \tilde{x}
 \mathbf{X}
 \hat{x}
 \overline{x}
 \dot{x}
 ∇
 ∇^s
 E^4
 0
 i

mix
atherm
 σ
c
EX
id
sat

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 D_i – Pseudobinary diffusivity of i $\left[\frac{m^2}{s}\right]$, 25
 E^4 – Axisymmetric Biharmonic Operator, 28
 F_B – Body Force $[N]$, 25
 H_V – Volumetric Energy Source $\left[\frac{W}{m^3}\right]$, 25
 J_i – Molar Diffusive species flux of i $\left[\frac{mol}{sm^2}\right]$, 25
 K_P – Pressure Equilibrium Constant Contribution $[varies]$, 26
 K_γ – Activity Coefficient Equilibrium Constant Contribution $[varies]$, 26
 K_ϕ – Fugacity Coefficient Equilibrium Constant Contribution $[varies]$, 26
 K_a – Equilibrium Constant $[varies]$, 26
 K_y – Mole Fraction Equilibrium Constant Contribution $[varies]$, 26
 M_W – Molecular Weight $\left[\frac{g}{mol}\right]$, 15, 26
 N_i – Mass Species Flux of i $\left[\frac{Kg}{m^2s}\right]$, 13, 16, 26, 33
 Q_N – Canonical Partition Function, 11, 12, 26
 Q_{cl} – Classical Partition Coefficient, 12, 26
 Q_{cm} – Center-of-Mass Partition Coefficient, 12, 26
 Q_{int} – Internal Partition Coefficient, 12, 26
 R_V – Volumetric Species Source $\left[\frac{mol}{sm^3}\right]$, 26
 S_A – Surface Area $[m^2]$, 26
 V_f – Free Volume $[m^3]$, 27
 Z^* – Configurational Integral $[none]$, 12, 27
 Δ – Isobaric/Isothermal Partition Function, 12, 15, 16, 27
 \Im – Degrees of Freedom $[none]$, 28
 Λ – DeBroglie Wavelength $[m]$, 12, 27
 Ω – Microcanonical Partition Function, 6, 10, 11, 28
 Ω_{mix} – Combinatorial Mixing Function $[none]$, 28
 Φ – Dissipation Function, 28
 Φ – Potential, 7, 8, 12, 13, 15, 28, 33
 $\Phi_{ij}(r)$ – Potential Function, 12, 13, 28
 Φ_n – FFT Basis Function, 28
 Π – Osmotic Pressure $[Pa]$, 14, 15, 27
 Ψ – Dimensionless Electric Potential $[none]$, 28
 Ψ – Stream Function $\left[\frac{m^2}{s}\right]$, 28
 Θ – Dimensionless Concentration or Temperature $[none]$, 27
 Θ_ν – Vibrational Frequency Factor, 27
 Θ_n – n^{th} FFT Coefficients, 27
 Ξ – Grand Canonical Partition Function, 11, 15, 27
 α – Thermal Diffusivity $\left[\frac{m^2}{s}\right]$, 27
 β – Boltzmann Normalization $\left[\frac{1}{J}\right]$, 9, 11–13, 27
 β – Thermal Expansion Coefficient $\left[\frac{1}{K}\right]$, 27
 β_i – Solute Expansion Coefficient due to species i $\left[\frac{1}{mol}\right]$, 27
 χ – Flory-Huggins Parameter $[none]$, 16, 28
 δ – Boundary Layer Thickness $[m]$, 6, 27
 ϵ – Dielectric Constant $\left[\frac{Coulombs^2}{Jm}\right]$, 6–8, 13, 27, 33
 $\epsilon_M, \epsilon_i, \epsilon_E$ – Eddy Diffusivity for Momentum, Species and Energy $\left[\frac{m^2}{s}\right]$, 27
 η – Intrinsic Viscosity $\left[\frac{m^3}{Kg}\right]$, 27

- η – heat cycle efficiency [none], 27
 γ – Surface Tension, CHANGE SIGMAS $[\frac{N}{m}]$, 14, 15, 27, 33
 γ_i – Activity Coefficient for species i [none], 27
 κ – COME BACK, 27
 λ – Debye Length [m], 27
 λ – Latent heat $[\frac{J}{mol}]$, 27
 λ – Wavelength [m], 27
 \dot{x} – Time derivative, 28
 \hat{f} – Mixture Fugacity, 25
 \hat{x} – Intensive Scalar, 28
 \tilde{x} – Extensive Vector, 28
 \mathcal{F} – Faraday's Constant, 28
 \mathcal{H} – Surface Mean Curvature, 25
 \mathcal{H}_i – Henry's Law Constant for specie i $[\frac{atm}{molfraction}]$, 25
 \mathcal{K}_i – Partition Coefficient [none], 25
 \mathcal{R} – Surface Reaction Rate, 28
 μ – Chemical Potential [J], 11, 14, 16, 27, 33
 μ – Viscosity [Pas], 27
 ν – Frequency $[\frac{1}{s}]$, 8, 27
 ν – Kinematic Viscosity $[\frac{m^2}{s}]$, 27
 ν_{ij} – Stoichiometric Coefficient for species i in reaction j , 27
 ν_i – Charge Valency of species i , 27
 ω – Accentricity Factor [none], 28
 ω – Microcanonical Partition Function, 10–12, 28
 ω_e – Electronic Degeneracy [none], 28
 \bar{x} – Partial Molar, 28
 ϕ – Electric Potential, 28
 ϕ – Fugacity Coefficient [none], 28
 ϕ_i – Flory-Huggins Mole Fraction of species i [none], 16, 28
 π – Constant, 12, 13, 15, 28
 ρ – Density $[\frac{Kg}{m^3}]$, 12, 13, 15, 27
 σ – Molecular Radius [A], 7, 8, 13, 28, 33
 σ – Symmetry Factor, 28
 σ – boundary, 6, 29, 33
 τ – Torque [Nm], 28
 τ_{ij} – Shear Rate in direction i perpendicular to j (CHECK FOR CONSISTENCY) $[\frac{N}{m^2}]$, 28
 \mathbf{X} – Matrix, 28
 \underline{S} – Stress Vector, 26
 $\underline{\nabla}$ – Gradient Operator, 28
 $\underline{\nabla}_s$ – Surface Gradient Operator, 28
 \underline{e} – Multicomponent Energy Flux, 25
 \underline{e}_i – Unit Vector in direction i [none], 25
 \underline{n} – Normal Vector [none], 26
 \underline{w} – Vorticity Vector, 27
 \underline{x} – Extensive Vector, 6, 28
 $\underline{\Gamma}$ – Rate-of-Strain Tensor, 27
 $\underline{\sigma}$ – Stress Tensor, 28
 \underline{w} – Vorticity Tensor, 27
 \underline{x} – Extensive Vector, 28
 \wp – Dynamic Pressure [Pa], 28
 ξ – Conjugate Coordinate, 27
 ξ – Extent of Reaction [none], 27
 c_D – Drag Coefficient [none], 25
 f – Fugacity, 6, 12, 25, 33
 $f_{\underline{e}_i}$ – Differential Force in direction of \underline{e}_i , 25
 k_B – Boltzmann Constant, 28
 $k_{c,i}$ – Mass Transfer Coefficient for species i $[\frac{mol}{sm^2conc.difference}]$, 25
 $q^{(x)}$ – Dufour Heat Flux, 26
 q_{elec} – Electronic Molecular Partition Coefficient, 12, 26
 q_{int} – Internal Molecular Partition Coefficient, 12, 26
 q_i – charge [Coulombs], 7, 26
 q_{nuc} – Nuclear Molecular Partition Coefficient, 12, 26
 q_{rot} – Rotational Molecular Partition Coefficient, 12, 26
 q_{trans} – Translational Molecular Partition Coefficient, 26
 q_{vib} – Vibrational Molecular Partition Coefficient, 12, 26
 x_i – i^{th} Conjugate Coordinate, 27
 x_i – Fraction of species i [none], 14–16, 27, 33
 z_i – Charge of species i [Coulombs], 27
 0 – Initial, 6, 15, 16, 28, 33
 a – Activity, 6, 8, 15, 16, 25, 33
 A – Helmholtz Energy [J], 11, 13, 25, 33
 $atherm$ – Athermal Function, 29
 B – Exergy [J], 9, 25
 B – Magnetic Induction $[\frac{Vs}{m^2}]$, 6, 25

- Bi – Biot Number *[none]*, 25
 Br – Brinkman Number *[none]*, 25
 C – Concentration $\left[\frac{\text{kg of } i}{\text{m}^3}\right]$, 14, 15, 25, 33
 c – Critical, 16, 29
 c – Speed of Light, 28
 D – Electric Displacement $\left[\frac{\text{Coulombs}}{\text{m}^2}\right]$, 6, 25
 Da – Damkohler Number *[none]*, 25
 e – Base of Natural Logarithm, 28
 E – Electric Field Strength $\left[\frac{\text{V}}{\text{m}}\right]$, 6, 25
 E – Energy $[J]$, 9–12, 25, 33
 EX – Excess Function, 15, 16, 29
 F – Force $[N]$, 6, 7, 25, 33
 G – Gibbs Energy $[J]$, 12, 15, 16, 25
 g – Gravitational Acceleration, 28
 g(r) – Radial Distribution Function *[none]*, 12, 13, 25
 Gr – Grashof Number *[none]*, 25
 H – Enthalpy $[J]$, 25
 h – Heat Transfer Coefficient $\left[\frac{\text{W}}{\text{m}^2\text{K}}\right]$, 25
 H – Magnetic Field Strength $\left[\frac{\text{A}}{\text{m}}\right]$, 6, 25
 h – Planck’s Constant, 12, 28
 i – Current Density $\left[\frac{\text{A}}{\text{m}^2}\right]$, 25
 I – Moment of Inertia $[Kg\text{m}^2]$, 25
 i – State or Level, COMPONENT?, 28
 id – Ideal Gas, 29
 K – Dilation Factor, 25
 K – Taylor Dispersion, 25
 k – Thermal Conductivity $\left[\frac{\text{W}}{\text{mK}}\right]$, 7, 9–13, 15, 25
 L – Length Scale $[m]$, 26
 m – Mass $[Kg]$, 12, 26
 mix – Mixing Function, 29
 N – Number of Moles *[none]*, 9–12, 14–16, 26, 33
 Nu – Nusselt Number *[none]*, 26
 P – Probability *[none]*, 9, 26
 P – Thermodynamic Pressure $[Pa]$, 6, 11, 12, 14, 15, 26
 Pe – Peclet Number *[none]*, 26
 Pr – Prandtl Number *[none]*, 26
 Q – Heat Flow $[W]$, 12, 26, 33
 q – heat flux $\left[\frac{\text{W}}{\text{m}^2}\right]$, 6, 26, 33
 R – Ideal Gas Constant, 8, 13–16, 28, 33
 r – Position $[m]$, 7, 8, 12, 13, 15, 26, 33
 Ra – Rayleigh Number *[none]*, 26
 Re – Reynolds Number *[none]*, 26
 S – Entropy $\left[\frac{J}{K}\right]$, 10, 26
 sat – Saturated Vapor, 29
 Sc – Schmidt Number *[none]*, 26
 Sh – Sherwood Number *[none]*, 26
 Sr – Strouhal Number *[none]*, 26
 T – Temperature $[K]$, 7, 9–16, 26
 t – Time $[s]$, 26
 u – Force Potential, 7, 26, 33
 U – Internal Energy $[J]$, 26
 U – Velocity $\left[\frac{\text{m}}{\text{s}}\right]$, 26
 v – Velocity $\left[\frac{\text{m}}{\text{s}}\right]$, 27
 V – Volume $[m^3]$, 6, 9–12, 14–16, 27, 33
 W – Work $[J]$, 6, 8, 27
 x – Displacement $[m]$, 6, 27, 33
 x – Extensive Scalar, 28
 Z – Compressibility *[none]*, 12, 27
 z – Height $[m]$, 27

5.6 Temporary Appendix - undeclared quantities

box number	undeclared symbol/s	uncertain symbol/s
1-1	none	F_f (force + fugacity) σ (boundary) \underline{q} (heat flux) \underline{V}_0 (volume + initial) F_x (force + displacement) x_0 (displacement + initial)
2-1	none	B_i (nth virial coefficient) \underline{E}_i (energy)
2-2	n_i	\tilde{N} (number of moles)
2-3	n_i	\tilde{N} (number of moles)
2-4	n_i	\tilde{N} (number of moles)
2-5	n_i	N (number of moles)
6-1	n	Q_{trans} (heat flow)
6-2	n	$\Phi(\underline{r}^N)$ (potential + position + number of moles)
		\underline{V}_f (volume + fugacity)
		N_A (mass species flux of i, + Helmholtz energy)
7-1	p	$\Phi(r)$ (potential + position) σ (molecular radius)
7-2	none	$u_{d-d}, u_{att}, u_{rep}$ (force potential) $\epsilon_{dipole}, \epsilon_{att}, \epsilon_{rep}$ (dielectric)
7-3	none	σ_{ij} (molecular radius) ϵ_{ij} (dielectric constant)
7-4	none	σ (molecular radius) R (ideal gas constant); $\Phi(r)$ (potential + position)
8-1	w, s, bar, pure, b_0	$C_s, C's$ (concentration) x_s, x_w (fraction of species i) μ_w (chemical potential) γ_w (surface tension) \bar{V}_w, \underline{V} (volume) B_2, B_3 (nth virial coefficient) N_i (mass species flux of i); Φ_{12} (potential) a_1 (activity)
8-2	n	μ_i (chemical potential) x_i (fraction of species i)