

# Index

- Acceptance-rejection algorithm, 231, 246, 316  
 Adiabatic relaxation, 297  
 Accommodation coefficient, 42, 321  
 Activation energy, 124, 267  
 Air, chemical rate coefficients for, 278, 283  
   collision model constants for, 294  
   equilibrium constants for, 124  
   vibrational rate constants for, 261  
 Angular momentum, 66  
 Arrhenius rate coefficient, 130, 269, 278, 281, 283  
 Atom-conservation, 112  
 Average velocity (*see* Bulk velocity)  
 Avogadro's number, 10, 154
- Backward reaction, 281  
 Bhatnagar, Gross, Krook (BGK) equation, 156  
 Bimodal distribution function, 212  
 Binary collision (*see* Collision)  
 Boltzmann constant, 10, 154  
 Boltzmann distribution, 95, 229, 315  
 Boltzmann equation, 22  
 Boltzmann limit, 92  
 Borgnakke-Larsen (BL) energy redistribution, 228, 245  
 Bose-Einstein statistics, 88  
 Boundary layer flow, 152  
 Breakdown parameter, 161, 186  
 Bulk velocity, 151, 339  
 Burnett equations, 47
- Calorically perfect gas, 11  
 Caloric equation of state, 11 (*see also* Perfect Gas)  
 Carbon dioxide, 241  
 Center-of-mass reference frame, 23, 330  
 Center-of-mass velocity, 23, 330  
 Chapman-Enskog theory, 155  
 Chapman-Enskog distribution function, BGK equation, 160  
   Boltzmann equation, 164  
 Characteristic density for dissociation, 122  
 Characteristic temperature, for dissociation, 121  
   for electronic excitation, 105  
   for rotation, 67, 253–256  
   for vibration, 67, 261  
 Chemical equilibrium, 121, 280, 296–304  
 Chemical nonequilibrium, 141, 277, 296–309  
 Chemical reactions, dissociation, 111, 267  
   exchange, 142, 280  
   recombination, 111, 287  
 Collision, binary, 22  
   dissociation, 133, 273, 333  
   elastic, 3, 204  
   exchange, 289, 334  
   gas-surface (*see* Gas-surface collisions)  
   inelastic, 3, 226  
   recombination, 289, 336  
   three-body, 289, 336  
 Collision cross-section (*see* Cross-section)  
 Collision frequency (*see* Collision rate)  
 Collision integral, 169, 178  
 Collision invariants, 29, 151, 157  
 Collision number, rotational, 227, 253–257  
   vibrational, 227, 259–262  
 Collision rate, 36, 197, 343  
 Collision quantities, 323  
 Collisionless flow (*see* Free molecular flow)  
 Computational grid strategies, 194  
 Conservation equations, for a single-species gas, 151  
   for gas mixtures, 166  
 Conservation, of energy, 151, 166  
   of mass, 151, 166  
   of momentum, 151, 166  
 Continuum breakdown parameter (*see* Breakdown parameter)  
 Continuum fluid equations (*see* Navier-Stokes equations)  
 Cross-section, differential, 24, 173  
   momentum, 174, 205, 216  
   total, 13, 174, 205, 216  
   viscosity, 173, 205, 216  
 Cross-section models, hard-sphere, 5, 204  
   generalized hard-sphere, 218  
   generalized soft-sphere, 218  
   variable hard-sphere, 204  
   variable soft-sphere, 216  
 Cumulative distribution function, 311

- Dalton's law of partial pressures, 114, 167, 342  
 Deflection angle, 175–177, 330–332  
 Degeneracy of quantum states, 60  
 Degrees of freedom, participating in a collision, 235–239  
   rotational, 111, 229  
   total, 268  
   translational, 111, 229, 327  
   vibrational, 109, 171, 225, 341  
 Detailed balance, 26  
 Diatomic gas, 107  
 Dilute gas, 22, 184, 189  
 Diffuse reflection (*see* Gas-surface collisions)  
 Diffusion (*see* Transport properties, mass transport)  
   binary coefficient of, 167–169, 174  
   coefficient of, 16, 171  
   self consistent effective binary diffusion (SCEBD) model for, 171  
   thermal coefficient of, 167  
 Diffusion velocity, 166  
 Direct simulation Monte Carlo (DSMC) method, 183  
 Dissociation energy (*see* Activation energy)  
 Dissociation reaction (*see* Chemical reactions)  
 Distribution function, definition of, 20  
   Chapman-Enskog, 164  
   Borgnakke-Larsen, 231, 246  
   for molecular speed, 32  
   for molecular velocity, 20  
   for quantized vibrational energy, 263–264  
   Maxwellian, 32  
   Maxwell-Boltzmann (*see* Maxwellian)  
 Drag, 44, 345  
  
 Elastic collisions (*see* Collision)  
 Electronic excitation, 72  
 Electron spin, 68  
 Energy, collision, 127, 268  
   electronic, 68  
   relative translational, 229, 329  
   rotational, 65, 229  
   translational, 9, 154  
   vibrational, 66, 263  
 Energy equation (*see* Conservation equations)  
 Energy levels (*see* Quantum energy states)  
 Enthalpy, 155, 167  
 Entropy, 84  
 Equation of state, caloric, 11  
   ideal gas, 10, 154  
 Equilibrium, chemical, 121, 280, 296–304  
   thermal, 7  
 Equilibrium constant, 124, 277  
 Equipartition of energy, 228  
 Error function, 347  
 Eucken's relation, 19, 171, 225  
 Euler equations, 45  
 Exchange reactions (*see* Chemical reactions)  
 Exclusion principle (*see* Pauli exclusion principle)  
  
 Fermi-Dirac statistics, 89  
 Fluctuations, real, 184, 187, 322  
   statistical, 199, 208, 322  
 Forward reaction, 280  
 Free energy (*see* Gibbs free energy)  
 Free molecular flow, 37–43, 48–50, 184  
 Frozen flow, 125  
  
 Gamma function, 347  
 Gas constant, ordinary or specific, 10, 154  
   universal, 10, 154  
 Gas-surface collisions, 42, 196, 320  
 Generalized hard-sphere (*see* Cross-section models)  
 Generalized soft-sphere (*see* Cross-section models)  
 Generalized post-energy redistribution, 245  
 Gradient length Knudsen number, 161, 186  
 Grad's moment equations, 155  
 Grid strategies (*see* Computational grid strategies)  
 Ground state, 61  
  
 Hard sphere (*see* Cross-section models)  
 Harmonic oscillator, 66  
 Heat flux vector (*see* Transport properties, energy transport)  
   from Chapman-Enskog analysis of the BGK equation, 162  
   from Chapman-Enskog analysis of the Boltzmann equation, 164  
   from kinetic theory, 161  
   for a monatomic mixture, 164  
   for a polyatomic mixture, 167  
   predicted by simulation, 345  
 Heisenberg's uncertainty principle, 56  
 Helmholtz free energy, 99  
 H-theorem, 26  
 Hypersonic limit, 40  
 Hypersonic flow simulations, 305  
  
 Ideal gas law (*see* Equation of state)  
 Impact parameter, 24, 173  
 Inelastic collision (*see* Collision)  
 Intermolecular forces (*see* Potential energy surface)  
 Intermolecular potential energy (*see* Potential energy surface)  
 Internal energy, 95  
   of the electronic mode, 105  
   of the rotational mode, 107  
   of the translational mode, 102  
   of the vibrational mode, 109  
 Inverse power law, 5, 176  
 Isothermal relaxation, 244, 258, 266, 294–304  
  
 Jeans equation for rotational relaxation, 126, 227

- Knudsen number, 160, 184  
 corresponding to the gradient length (*see* Gradient length Knudsen number)
- Landau-Teller equation for vibrational relaxation, 126, 227
- Larsen-Borgnakke (*see* Borgnakke-Larsen (BL) energy redistribution)
- Law of mass action, 113
- Lennard-Jones potential, 178
- Liouville equation, 48
- Loschmidt's number, 184
- Mach number, 51, 160
- Macrostate, 87
- Mass density, 7, 167
- Mass fraction, 121, 172
- Mass transport (*see* Transport properties)
- Maxwellian distribution, 29, 313
- Mean collision time, 343
- Mean free path, 12, 184, 343
- Mean molecular speed (*see* Mean thermal speed)
- Mean velocity (*see* Bulk Velocity)
- Mean thermal speed, 37
- Mechanical equilibrium (*see* Equilibrium)
- Microstate, 87
- Millikan-White vibration model, 128, 260
- Mixture of gases, chemical rate equation for, 129  
 collision rate of, 36, 343  
 DSMC collision rate algorithm for, 201  
 diffusivity of, 167, 171  
 evaluating macroscopic properties of, 341  
 equilibrium properties of, 111  
 mass velocity of, 166, 341  
 thermal conductivity of, 171  
 viscosity of, 170
- Molecular collisions (*see* Collisions)
- Molecular dynamics (MD) method, 183, 214
- Molecular magnitudes, 184
- Moment of a distribution function, 21, 150
- Momentum equations (*see* Conservation equations)
- Momentum transport (*see* Transport properties)
- Monatomic gas, 11
- Morse potential, 77
- Most probable speed (*see* Speed)
- Navier-Stokes equations, 46, 155, 166
- Nitric oxide (*see* Air)
- Nitrogen (*see* Air)
- Nonequilibrium, chemical, 141, 267, 277, 293–309  
 mechanical, 212  
 thermal, 252, 259
- No-Time-Counter (NTC) collision rate algorithm, 197
- Normal shock wave (*see* Shock wave)
- Number density, 6
- Oxygen (*see* Air)
- Park five species air reaction model, 278
- Park vibrational relaxation parameters, 261
- Parker rotation model, 129, 253
- Partial pressure (*see* Dalton's law of partial pressures)
- Particle model, 4
- Particle movement, 193
- Particle sorting, 193
- Particle selection procedures, 236
- Particle weight, 197
- Partition function, electronic, 104  
 rotational, 107, 280  
 translational, 99, 280  
 vibrational, 108, 280
- Pauli exclusion principle, 69
- Peculiar velocity, 151, 166
- Perfect gas (*see* Ideal gas law)
- Phase space, 22
- Photon, 54
- Planck's constant, 54
- Poisson distribution, 199
- Polyatomic gas, 19, 165, 241
- Potential energy function (*see* Potential energy surface)
- Potential energy surface (PES), 150, 178
- Prandtl number, 19, 162, 164
- Pressure, dilute gas, 153, 167  
 on a wall, 7, 345
- Pressure tensor, 152
- Quantum energy states, electronic, 68  
 rotation, 65  
 translation, 60  
 vibration, 66, 263
- Quantum mechanics, 54
- Quantum number, 60
- Quasi steady state (QSS), 295–304
- Random number, 311
- Random thermal velocity (*see* Peculiar velocity)
- Rate coefficient, 130  
 for chemically reacting air species, 278
- Rate equation (*see* Mixture of gases, chemical rate equation for)
- Ratio of specific heats, 11
- Ray tracing algorithm, 196
- Recombination reactions (*see* Chemical reactions)
- Reduced mass, 23
- Relative speed (*see* Relative velocity)
- Relative velocity, 23, 197, 329
- Relative velocity vector, 330–332
- Relaxation time, rotational, 118, 227, 253  
 vibrational, 118, 227, 260
- Root-mean-square molecular speed (*see* Speed)

- Scattering angle (*see* Deflection angle)  
 post-collision algorithms for, 329
- Schmidt number, 206, 217
- Schrodinger equation, 57
- Self consistent effective binary diffusion (SCEBD), 171
- Shear stress tensor (*see* Transport properties, momentum transport)
- Shock wave, simulation results for, 210, 212, 222, 305
- Simple Gas, 4
- Slip velocity (*see* Velocity slip)
- Sonine polynomials, 163
- Specific heats, 11
- Specular reflection (*see* Gas-surface collisions)
- Speed, average molecular, 33  
 most probable molecular, 33  
 root-mean-square molecular, 34
- Speed of sound, 160
- Speed ratio, 39
- Statistical fluctuations (*see* Fluctuations)
- Statistical mechanics, 84
- Stefan-Maxwell equations, 167
- Steric factor, 134, 270
- Stirling's formula, 90
- Subsonic simulation boundary conditions, 322
- Temperature, average, 340, 342  
 translational, 154, 340, 342  
 rotational, 340, 342  
 vibrational, 340, 342
- Temperature jump, 47, 321
- Thermal conductivity (*see* Transport properties, energy transport)  
 for a monatomic mixture, 164  
 for a polyatomic mixture, 171
- Thermal equilibrium (*see* Equilibrium)
- Thermal velocity (*see* Peculiar velocity)
- Thermodynamics, link with statistical mechanics, 84
- Three-body collision (*see* Collision)
- Time constants (*see* Relaxation time)
- Total collision energy (TCE) model, 267
- Transition regime, 51, 184
- Transport properties, general discussion of, 14  
 mass transport and diffusion coefficient, 15, 166–172  
 momentum transport and viscosity coefficient, 16, 161, 164, 167, 170  
 energy transport and thermal conductivity coefficient, 16, 161, 164, 167, 171
- Uncertainty principle (*see* Heisenberg's uncertainty principle)
- Variable hard sphere (*see* Cross-section models)
- Variable soft sphere (*see* Cross-section models)
- Velocity distribution function (VDF), 20, 212
- Velocity slip, 47, 321
- Velocity space (*see* Phase space)
- Vibrationally favored dissociation (VFD) model, 276
- Viscosity (*see* Transport properties, momentum transport)  
 from Chapman-Enskog analysis of the BGK equation, 162  
 from Chapman-Enskog analysis of the Boltzmann equation, 164  
 for a monatomic mixture, 169  
 for a polyatomic mixture, 170
- Viscous stress tensor (*see* Transport properties, momentum transport)
- Wave function, 57
- Zero-point energy, 112