Bahman Zohuri · Patrick McDaniel

Combined Cycle Driven Efficiency for Next Generation Nuclear Power Plants

An Innovative Design Approach

 Second Edition

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ISBN 978-3-319-70550-7 ISBN 978-3-319-70551-4 (eBook) <https://doi.org/10.1007/978-3-319-70551-4>

Library of Congress Control Number: 2017959326

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Printed on acid-free paper

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This book is dedicated to my children Natasha, Natalie, and Sasha as well as my grandson Darius. They always encouraged me with my publications.

Bahman Zohuri

I would like to dedicate this book to my wife Nancy Lee Ries who provided many years of inspiration for my work.

Patrick McDaniel

Preface to the Second Edition

The second edition includes what was presented in the first edition, while also presenting a revised version of Chap. [9](#page--1-0) based on new investigation and analysis, which were done by modifying the existing computer code, namely, combined cycle (CC).

As discussed in Chap. [9,](#page--1-0) since the CC code performs well at modeling current generation combined cycle gas turbine (CCGT) plants, it is useful to extrapolate its capabilities to Nuclear Air-Brayton Combined Cycle (NACC) power plants and Nuclear Air-Brayton Recuperated Cycle (NARC) power plants. The combined cycle plants are dealt with in Chap. [9](#page--1-0) and the recuperated plants in Chap. [10](#page--1-0). In Nuclear Air-Brayton power plants, the combustion chamber of the gas turbine system is replaced by the nuclear reactor and a heat exchanger. The nuclear reactor will heat a working fluid, and that working fluid will in turn pass through a heat exchanger to heat the air for the turbine. Because the heat transfer process for a nuclear system is in the opposite direction (solid to gas) from that in the gas turbine (gas to solid), the peak temperatures achievable in a Nuclear Air-Brayton system will never be as high as those in a gas turbine system. However, the nuclear system can reheat the air multiple times and expand it across multiple turbines to increase the available power.

In comparing nuclear systems, there are multiple advantages for the Nuclear Air-Brayton cycle over conventional light water cycles. The ability to go to higher temperatures while not being trapped under the water vapor dome adds a major flexibility. The higher gas temperatures allow for the implementation of a combined cycle approach to improve system efficiency. There is also a much larger base of gas turbine manufacturers than large steam turbine manufacturers for system designers to draw from. All downstream components after the turbines themselves are currently being used in GTCC plants. A NACC plant will require significantly less water for waste heat removal than a current light water reactor (LWR) system because the efficiency is greater and a significant amount of the waste heat is directly dumped into the atmosphere without going through a cooling tower.

Finally, the NARC system dumps all of its heat into the atmosphere and as a result is not tied to a location near a water source. In addition to Chap. [9](#page--1-0), a new Chap. [10](#page--1-0) is written for the second edition, which explains the Nuclear Air-Brayton Recuperated Cycle (NARC). Its biggest advantage is that the simple recuperated cycle is not tied to a water source. The NARC power plant is not tied to a seacoast or river valley.

Currently, the largest power station in the United States, Palo Verde, is restrained from expanding, not for any safety reason, but for lack of additional fresh water to dump its waste heat. In the recuperated cycle, a heat exchanger is placed in the exhaust from the last turbine, and instead of transferring heat to water as a working fluid, it transfers its heat to the air exiting the compressor to preheat it before it enters the first sodium-, or molten salt-, to-air heat exchanger. It is possible to split the compressor and add an intercooler to improve the efficiency of the recuperated cycle. This allows more heat to be extracted from the exhaust stream with the recuperator. In both chapters, the results of computer code CC calculation are replotted for better understating of new modification of the code CC and its capabilities.

In the second edition, significant new results have become available for intercooled systems. Technology plans can now be described for connecting a Nuclear Air-Brayton as an online storage system for a low-carbon grid.

The first edition has a minor error in one of the steam tables near the critical point. This is not likely to affect any engineered system, but it would be better to have the correct data in the table.

Albuquerque, New Mexico, USA Bahman Zohuri September 26, 2017 **Patrick McDaniel**

Preface to the First Edition

Today's global energy market places many demands on power generation technology including high thermal efficiency, low cost, rapid installation, reliability, environmental compliance, and operation flexibility.

The demand for clean, non-fossil-based electricity is growing; therefore, the world needs to develop new nuclear reactors with higher thermal efficiency in order to increase electricity generation and decrease the detrimental effects on the environment. The current fleet of nuclear power plants is classified as Generation III or less. However, these models are not as energy efficient as they should be because the operating temperatures are relatively low. Currently, groups of countries have initiated an international collaboration to develop the next generation of nuclear reactors called Generation IV. The ultimate goal of developing such reactors is to increase the thermal efficiency from what currently is in the range of 30–35% to 45–50%. This increase in thermal efficiency would result in a higher production of electricity compared to current pressurized water reactor (PWR) or boiling water reactor (BWR) technologies.

A number of technologies are being investigated for the Next Generation Nuclear Plant that will produce heated fluids at significantly higher temperatures than current generation power plants. The higher temperatures offer the opportunity to significantly improve the thermodynamic efficiency of the energy conversion cycle. One of the concepts currently under study is the molten salt reactor (MSR). The coolant from the molten salt reactor may be available at temperatures as high as 800–1000 °C. At these temperatures, an open Brayton cycle combined with Rankine bottoming cycle appears to have some strong advantages.

Combined-cycle thermal efficiency increases as gas turbine specific power increases. The gas turbine firing temperature is the primary determinant of specific power.

Gas turbine engines, both aircraft and industrial power generation, represent one of the most aggressive applications for structural materials. With ever-growing demands for increasing performance and efficiencies, all classes of materials are being pushed to higher temperature capabilities. These materials must also satisfy stringent durability and reliability criteria. As materials are developed to meet these demanding requirements, the processing of these materials often becomes very complicated and expensive. As a result, the cost of materials and processes has become a much larger consideration in the design and application of highperformance materials. Both the aircraft engine and power generation industries are highly cost competitive, and market advantage today relies on reducing cost as well as increasing performance and efficiency.

Development of high-temperature/high-strength materials, corrosion-resistant coatings, and improved cooling technology has led to increases in gas turbine firing temperatures. This increase in firing temperature is the primary development that has led to increases in combined cycle gas turbine (CCGT) thermal efficiencies. The improvements in combined cycle thermal efficiencies and the commercial development of combined cycle power plants have proceeded in parallel with advances in gas turbine technologies.

The Generation IV International Forum (GIF) program has narrowed design options of the nuclear reactors to six concepts. These concepts are gas-cooled fast reactor (GFR), very-high-temperature reactor (VHTR), sodium-cooled fast reactor (SFR), lead-cooled fast reactor (LFR), molten salt reactor (MSR), and supercritical water-cooled reactor (SCWR). These nuclear reactor concepts differ in their design in aspects such as the neutron spectrum, coolant, moderator, and operating temperature and pressure.

There are many different types of power reactors. What is common to them all is that they produce thermal energy that can be used for its own sake or converted into mechanical energy and ultimately, in the vast majority of cases, into electrical energy. Thermal-hydraulic issues related to both operating and advanced reactors are presented. Further thermal-hydraulic research and development is continuing in both experimental and computational areas for operating reactors, reactors under construction or ready for near-term deployment, and advanced Generation IV reactors. As the computing power increases, the fine-scale multi-physics computational models, coupled with the systems analysis code, are expected to provide answers to many challenging problems in both operating and advanced reactor designs.

Compact heat exchangers, filters, turbines, and other components in integrated Next Generation Nuclear Plant combined cycle system must withstand demanding conditions of high temperatures and pressure differentials. Under the highly sulfiding conditions of the high temperature such as inlet hot steam or other related environmental effects, the performance of components degrades significantly with time unless expensive high-alloy materials are used. Deposition of a suitable coating on a low-cost alloy may improve its resistance to such sulfidation attack and decrease capital and operating costs. A review of the literature indicates that the corrosion reaction is the competition between oxidation and sulfidation reactions. The Fe- and Ni-based high-temperature alloys are susceptible to sulfidation attack unless they are fortified with high levels of Cr, Al, and Si. To impart corrosion

resistance, these elements need not be in the bulk of the alloy and need only be present at the surface layers.

Those that practice the art of nuclear engineering must have a physical and intuitive understanding of the mechanisms and balances of forces, which control the transport of heat and mass in all physical systems. This understanding starts at the molecular level, with intermolecular forces and the motion of molecules, and continues to the macroscopic level where gradients of velocity, temperature, and concentration drive the diffusion of momentum, heat, and mass and the forces of pressure, inertia, and buoyancy balance drive convection of fluids.

This text covers the fundamentals of thermodynamics required to understand electrical power generation systems. It then covers the application of these principles to nuclear reactor power systems. It is not a general thermodynamics text, but is a thermodynamics text aimed at explaining the fundamentals and applying them to the challenges facing actual nuclear power systems. It is written at an undergraduate level, but should also be useful to practicing engineers.

Chapters [3](#page--1-0) and [4](#page--1-0) are provided by Professor Bill Garland of the Department of Engineering Physics at McMaster University Ontario, Canada, and his permission was given to the author exclusively to use the lecture, class notes, and other related materials that he wrote during the time he was teaching at the university.

The book also concentrates on fundamentals of fluid dynamics and heat transfer, thermal and hydraulic analysis of nuclear reactors, two-phase flow and boiling, compressible flow, stress analysis, and energy conversion methods.

The book presents the fundamental definitions of units and dimensions; thermodynamic variables such as temperature, pressure, and specific volume; thermalhydraulic analysis with the topics in that field from Chaps. [2](#page--1-0) through [16](https://doi.org/10.1007/978-3-319-70551-4_16); design of heat exchanger and shell and tube using a different verification and validation (V&V) in computational mechanics; and applications of the fundamentals to Brayton and Rankine cycles for power generation. Brayton cycle compressors, turbines, and recuperators are covered, in general, along with the fundamentals of heat exchanger design. Rankine steam generators, turbines, condensers, and pumps are discussed. Reheaters and feedwater heaters are also covered. Ultimate heat rejection by circulating water systems is also discussed. Chapter [17](https://doi.org/10.1007/978-3-319-70551-4_17) covers the analysis of reactor accidents, which is independent from other chapters and can be assigned as a standalone reading chapter for a student or independently be taught.

The third part of the book covers current and projected reactor systems and how the thermodynamic principles are applied to their design, operation, and safety analyses.

Detailed appendices cover metric and English system units and conversions, detailed steam and gas tables, heat transfer properties, and nuclear reactor system descriptions.

Albuquerque, New Mexico, USA Bahman Zohuri

Patrick McDaniel

Acknowledgments

We would like to acknowledge all those who helped, encouraged, and supported us in our work. We have decided not to name them all since some of them may not be around to see the end result of their encouragement, but we hope they can at least read this acknowledgment wherever they may be.

Last but not least, special thanks are given to our parents, wives, children, and friends for providing constant encouragement, without which this book could not have been written. We especially appreciate their patience with our frequent absences from home and long hours in front of the computer during the preparation of this book.

Contents

About the Authors

Dr. Bahman Zohuri is currently at the Galaxy Advanced Engineering, Inc., a consulting company that he started himself in 1991 when he left both semiconductor and defense industries after many years working as a chief scientist. He is also presently holding the position of research professor at the Department of Electrical and Computer Engineering at the University of New Mexico. After graduating from the University of Illinois in the field of physics and applied mathematics, he joined the Westinghouse Electric Corporation where he performed thermal-hydraulic analysis and natural circulation for inherent shutdown heat removal system (ISHRS) in the core of a liquid metal fast breeder reactor (LMFBR) as a secondary fully inherent shut system for secondary loop heat exchange. All these designs were used for nuclear safety and reliability engineering for self-actuated shutdown system. He designed the mercury heat pipe and electromagnetic pumps for large pool concepts of LMFBR for heat rejection purpose for this reactor in around 1978 where he received a patent for it. He later on was transferred to the defense division of Westinghouse where he was responsible for the dynamic analysis and method of launch and handling of MX missile out of canister. He later on was consultant at Sandia National Laboratories (SNL) after leaving the United States Navy. Dr. Zohuri earned his bachelor's and master's degrees in physics from the University of Illinois and his second master's degree in mechanical engineering as well as his doctorate in nuclear engineering from the University of New Mexico. He has been awarded three patents and has published 26 textbooks and numerous other journal publications.

He did few years of consulting under his company Galaxy Advanced Engineering, Inc., with Sandia National Laboratories (SNL), where he was supporting the development of operational hazard assessments for the Air Force Safety Center (AFSC) in connection with other interested parties. Intended use of the results was their eventual inclusion in Air Force Instructions (AFIs) specifically issued for directed-energy weapon (DEW) operational safety. He completed the first version of a comprehensive library of detailed laser tools for Airborne Laser (ABL), Advanced Tactical Laser (ATL), Tactical High-Energy Laser (THEL), Mobile/ Tactical High-Energy Laser (M-THEL), etc.

He also was responsible for SDI computer programs involved with Battle Management and C3I (Command, Control, Communication and Intelligent) and artificial intelligent and autonomous system. He is author few publications and holds various patents such as laser-activated radioactive decay and results of thrubulkhead initiation.

Recently, he has published over 23 other books with Springer Publishing Company and CRC and Taylor & Francis on different subjects, and they all can be found under his name on Amazon.

Dr. Patrick McDaniel is currently adjunct and research professor at the Department of Chemical and Nuclear Engineering, University of New Mexico. Patrick began his career as a pilot and maintenance officer in the USAF. After leaving the Air Force and obtaining his doctorate at Purdue University, he worked at Sandia National Laboratories in fast reactor safety, integral cross section measurements, nuclear weapon vulnerability, space nuclear power, and nuclear propulsion. He left Sandia to become the technical leader for Phillips Laboratory's (became part of the Air Force Research Laboratory) Satellite Assessment Center. After 10 years at PL/AFRL, he returned to Sandia to lead and manage DARPA's Stimulated Isomer Energy Release project, a \$10 M per year effort. While at Sandia, he worked on the Yucca Mountain Project and DARPA's classified UER-X program. Having taught at the University of New Mexico in the graduate nuclear engineering program for 25 years, when he retired from Sandia in early 2009, he joined the faculty at the University of New Mexico full time. He has worked on multiple classified and unclassified projects in the application of nuclear engineering to high energy systems. Dr. McDaniel holds a PhD in nuclear engineering from Purdue University. Dr. McDaniel is a research professor at the Nuclear Engineering Department of University of New Mexico at the present time.

Chapter 1 Definitions and Basic Principles

Nuclear power plants currently generate better than 20% of the central station electricity produced in the United States. The United States currently has 104 operating power-producing reactors, with 9 more planned. France has 58 with 1 more planned. China has 13 with 43 planned. Japan has 54 with 3 more planned. In addition, Russia has 32 with 12 more planned. Nuclear-generated electricity has certainly come into its own existence and is the safest, cleanest, and greenest form of electricity currently produced on this planet. However, many current thermodynamic texts ignore nuclear energy and use few examples of nuclear power systems. Nuclear energy presents some interesting thermodynamic challenges, and it helps to introduce them at the fundamental level. Our goal here will be to introduce thermodynamics as the energy conversion science that it is and apply it to nuclear systems. Certainly, there will be many aspects of thermodynamics that are given little or no coverage. However, that is true for any textual introduction to this science; however, by considering concrete systems, it is easier to give insight into the fundamental laws of the science and to provide an intuitive feeling for further study [[1\]](#page--1-0).

1.1 Typical Pressurized Water Reactor

By far the most widely built nuclear system is the pressurized water reactor (PWR). There are a number of reasons for this. Steam turbines have for many decades been the dominant means of generating mechanical energy to turn electrical generators. The temperatures reached in the thermodynamic cycle of a PWR are within the range of fairly, common engineering materials. They were the first system built and operated reliably to produce electricity. A typical PWR system is described in Fig. [1.1.](#page-19-0)

The basic PWR consists of five major components, the reactor core, steam generator(s), steam turbine, condenser, and electrical generator and three water/

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B. Zohuri, P. McDaniel, Combined Cycle Driven Efficiency for Next Generation Nuclear Power Plants, https://doi.org/10.1007/978-3-319-70551-4_1

Fig. 1.1 Pressurized water reactor schematic

steam loops. Each loop requires a pump that is not shown to keep the diagram cleaner. The nuclear energy is converted to thermal energy in the reactor core. This thermal energy is then transported via the first loop to the steam generator where it is passed to the water in the second loop. The water in the second loop enters as a liquid and is turned to steam. The steam then passes to the turbine where the thermal energy is converted to mechanical energy to rotate the electrical generator. After the thermal energy has been converted to mechanical energy in the steam turbine, the low-pressure steam passes to the condenser to be cooled by the water in the third loop. The second law of thermodynamics tells us that we cannot simply expand the steam to a low enough energy state that it can return to the steam generator in its original liquid state. Therefore, we must extract more thermal energy from the low-pressure steam to return it to its liquid state where it can be pumped back into the steam generator. The third loop is called the circulating water system and it is open to the environment. There are multiple ways of providing this cooling water including intake and return to a river, or the ocean, intake and return to a cooling pond, or intake from a river and exhaust through a cooling tower. However, we are getting ahead of ourselves.

Consider for a minute why nuclear energy is so useful. A great deal of energy is produced by a very little mass.

Example Calculation: Calculate the U-235 consumed to produce 1 MW of thermal energy for 1 day. Note that a megawatt is a unit of power, or energy per unit time:

1 MW = 10^6 watts = 10^6 joules/s 1 day = 24 hours = $24*3600$ s

The energy released in fission of a U-235 atom is \sim 200 Mev:

 $1 \text{ ev} = 1.6 \times 10^{-19} \text{ joules } 1 \text{ Mev} = 1.6 \times 10^{-13} \text{ joules } 200 \text{ Mev} = 32 \text{ picojoules}$ Fissioning 1 atom of U-235 produces 3.2×10^{-11} joules.

To produce 10⁶ joules requires $106/3.2 \times 10^{-11}$ atoms = 3.125 \times 10¹⁶ atoms.

And for a duration of 8.64 \times 10⁴ s, the total number of atoms consumed will be $3.125 \times 8.64 \times 10^{20}$ atoms.

Therefore 2.7×10^{21} atoms will be consumed. A gram mole of U-235 is 6.022×10^{23} atoms.

So a gram is $6.022 \times 10^{23} / 235 = 2.563 \times 10^{21}$ atoms/gram.

Therefore 1 megawatt-day of nuclear energy consumes 1.05 grams of U-235.

The fundamental thing to understand is that a PWR converts nuclear energy to electrical energy, and it does this by converting the nuclear energy first to thermal energy and then converting the thermal energy to mechanical energy, which is finally converted to electrical energy. The science of thermodynamics deals with each of these conversion processes. To quantify how each of these processes takes place, we must understand and apply the laws of thermodynamics.

1.2 Scope of Thermodynamics

Thermodynamics is the science that deals with energy production, storage, transfer, and conversion. It is a very broad subject affects most fields of science including biology and microelectronics. The primary forms of energy considered in this text will be nuclear, thermal, chemical, mechanical, and electrical. Each of these can be converted to a different form with widely varying efficiencies. Predominantly thermodynamics is most interested in the conversion of energy from one form to another via thermal means. However, before addressing the details of thermal energy conversion, consider a more familiar example. Newtonian mechanics defines work as force acting through a distance on an object. Performing work is a way of generating mechanical energy. Work itself is not a form of energy, but a way of transferring energy to a mass. So when one mass gains energy, another mass, or field, must lose that energy.

Consider a simple example. A 65-kg woman decides to go over Niagara Falls in a 25-kg wooden barrel. (The first person to go over the fall in a barrel was a woman, Annie Taylor.) Niagara Falls has a vertical drop of 50 m and has the highest flow rate of any waterfall in the world. The force acting on the woman and barrel is the force of gravity, which at the surface of the earth produces a force of 9.8 Newton for every kilogram of matter that it acts on. So we have

$$
W = F \times D \qquad F = (65 + 25) \times 9.8 = 882.0
$$
 Newton $D = 50$ m
$$
W = 882.0 \times 50.0 = 44,100
$$
Newton-meters = 44.1 kilojoules

A Newton-meter is a joule and 1000 joules is a kilojoule. Therefore, when the woman and barrel went over the falls, by the time they had reached the bottom, the force of gravity had performed 44.1 kilojoules (kJ) of work on them. The gravitational field had 44.1 kJ of potential energy stored in it, when the woman and the barrel were at the top of the falls. This potential energy was converted to kinetic energy by the time the barrel reached the bottom of the falls. Kinetic energy is also measured in joules, as with all other forms of energy. However, we are usually most interested in velocities when we talk about kinetic energies, so let us extract the velocity with which she hit the waters of the inlet to Lake Ontario.

$$
\Delta KE = \Delta PE = 44.1 \,\text{kJ} = 1/2 \,\text{mV}^2 = (90/2) \,\text{kg} \times V^2 \quad V^2 = 44.1 \,\text{kJ} / (90/2) \,\text{kg}
$$

Now it is a matter of converting units. A joule is a Newton-meter. 1 Newton is defined as 1 kg accelerated at the rate of 1 meter/second/second. So,

44.1 kJ = 44, 100 Newton-meters
= 44, 100 kilogram meter/sec / sec -meter
= 44, 100 kilogram
$$
(m/s)^2
$$

$$
V^2 = 44,100 \text{ kg}(\text{m/s})^2/(90/2) \text{kg}
$$

= 490/(1/2) = 980(m/s)²

$$
V = 31.3 \text{ m/s } (\text{70 mph})
$$

Needless to say, she recommended that no one ever try that again. Of course, others have, some have made it, and some have drowned.

Before leaving this example, it is worth pointing out that when we went to calculate the velocity, it was unaffected by the mass of the object that had dropped the 50 m. So one half the velocity squared represents what we will call a specific energy, or energy per kilogram. In addition, the potential energy at the top of the falls could be expressed as a specific potential energy relative to the waters below. The potential energy per pound mass would just be the acceleration of gravity times the height of the falls. Typically, we will use lowercase letters to represent specific quantities and uppercase letters to represent extensive quantities. Extensive quantities are dependent upon the amount of mass present. Specific quantities are also referred to as intensive variables, though there are some intensive variables that have no extensive counterpart, such as pressure or temperature:

$$
p.e. = mgh/m = gh = 9.8 \times 50 = 0.49 \text{ kJ/kg}
$$

It is also worth pointing out that Newton's law of gravity states that

$$
F = G \frac{m_1 M_2}{R^2} \tag{1.1}
$$

where m_1 is the smaller mass and M_2 is the mass of the Earth. We can find the specific force on an object by dividing the gravitational force by the mass of the object. For distances like 50 m on the surface of the Earth $(R = 6, 378, 140 \,\text{m})$, we can treat R as constant, but if the distance the gravitational force acts through is comparable to the radius of the Earth, an integration would be required. Even on the top of Mount Everest, the gravitational potential is within 0.25% of that at sea level, so gravity is essentially constant for all systems operating on the face of the Earth.

1.3 Units

In this section, we will discuss the System International (SI) and English (E) systems.

1.3.1 Fundamental Units

Before going further, it will be a very good idea to discuss units for physical quantities and the conversion of units from one system to another. Unfortunately, the field of thermodynamics is beset with two popular systems of units. One is the System International (SI) system consisting of the kilogram, meter, and second. The other is the English (E) system consisting of the pound mass, foot, and second.

Starting with the SI system, the unit of force is the Newton. The unit of work or energy is the joule and the unit of pressure is the pascal. We have

> $1 N = 1$ kilogram-meter/s² 1 joule $=$ 1 Newton-meter 1 pascal = 1 Newton/m²

Now the acceleration of gravity at sea level on Earth is 9.8066 m/s^2 , so a 100 kg mass will weight 980.66 Newton. Also when we want avoid spelling out very large or small quantities, we will usually use the standard abbreviations for powers of 10 in units of 1000. We have

```
kilo = 10<sup>3</sup>mega = 10^6giga = 10^9deci = 10^{-1}centi = 10^{-2}milli = 10^{-3}micro = 10^{-6}nano = 10^{-9}
```
For the English system, we have

 $lbm \implies 1$ lbf (at Sea Level) $1 \text{ ft} - \text{lbf} = 1 \text{ lbf} \times 1 \text{ ft}$ 1 British Thermal Unit $(BTU) = 778$ ft -1 bf 1 psi = 1 lbf/in^2

Note that the fact that 1 lbf $=$ 1 lbm at sea level on Earth means that a mass of 100 lbm will weigh 100 lbf at sea level on Earth. The acceleration of gravity at sea level on Earth is 32.174 feet/s². Thus, we have 1 lbf/(1 lbm-foot/s²) = 32.174. If we

move to another planet where the acceleration of gravity is different, the statement that $1 \text{ lbm} > 1 \text{ lbf doesn't hold.}$

Consider comparative weights on Mars. The acceleration of gravity on Mars is 38.5% of the acceleration of gravity on Earth. So in the SI system we have

$$
W = 0.385^* \, 9.8066 \, \text{m/s}^2 \times 100 \, \text{kg} = 377.7 \, \text{Newton}
$$

In the English system, we have

$$
W = 0.385^* \, 100 \, \text{lbm} = 38.5 \, \text{lbf}
$$

1.3.2 Thermal Energy Units

The British thermal unit (Btu) is defined to be the amount of heat that must be absorbed by a 1 lb-mass to raise its temperature $1^{\circ}F$. The calorie is the SI unit that is defined in a similar way. It is the amount of heat that must be absorbed by 1 gram of water to raise its temperature $1 \,^{\circ}\text{C}$. This raises the question as to how a calorie compares with a joule since both appear to be measures of energy in the SI system. James Prescott Joule spent a major part of his life proving that thermal energy was simply another form of energy like mechanical kinetic or potential energy. Eventually his hypothesis was accepted and the conversion factor between the calorie and joule has been defined by

1 calorie $= 4.1868$ Joules

The constant 4.1868 is called the mechanical equivalent of heat.

1.3.3 Unit Conversion

As long as one remains in either the SI system or the English system, calculations and designs are simple. However, that is no longer possible as different organizations and different individuals usually think and work in their favorite system. In order to communicate with an audience that uses both SI and English systems, it is important to be able to convert back and forth between the two systems. The basic conversion factors are

 $1 \text{ kg} = 2.204621$ bm $1 \text{ lbm} = 0.45359 \text{ kg}$ 1 meter $= 3.2808$ feet 1 foot $= 0.3048$ meter 1 joule $= 0.00094805$ Btu $1 \text{Btu} = 1055$ joules $1 atm = 14.696 \,\text{psi}$ $1 atm = 101325 pascal$ $1 \text{ psi} = 6894.7 \text{ pascal}$ $1 bar = 100000.0 pascal$ $1 bar = 14.504 \,\text{psi}$

The bar unit is simply defined by rounding off sea level atmospheric pressure to the nearest 100 kilopascal. There are many more conversion factors defined in the Appendix, but they are all derived from this basic few.

1.4 Classical Thermodynamics

Classical thermodynamics was developed long before the atomic theory of matter was accepted. Therefore, it treats all materials as continuous and all derivatives well defined by a limiting process. Steam power and an ability to analyze it and optimize it was one of the main drivers for the development of thermodynamic theory. The fluids involved always looked continuous. A typical example would be the definition of the density of a substance at a point. We have,

$$
\rho = \lim_{\Delta V \to 0} \frac{\Delta m}{\Delta V} \tag{1.2}
$$

As long as ΔV does not get down to the size of an atom, this works. Since classical thermodynamics was developed, however, we have come to understand that all gases and liquids are composed of very small atoms or molecules and a limiting process that gets down to the atomic or molecular level will eventually become discontinuous and chaotic. Nevertheless, the continuous model still works well for the macroscopic systems that will be discussed in this text, and classical thermodynamics is based on it.

At times, we will refer to an atomistic description of materials in order to develop a method of predicting specific thermodynamic variables that classical thermodynamics cannot predict. A typical example is the derivative that is called the constant volume-specific heat. This variable is defined as the rate of change of the internal energy stored in a substance as a function of changes in its temperature. Classical thermodynamics demonstrates that this variable has to exist and makes great use of it, but it has no theory for calculating it from first principles. An atomistic view will allow us to make some theoretical estimates of its value. Therefore, at times we will deviate from the classical model and adopt an atomistic view that will improve our understanding of the subject.

Classical thermodynamics is also an equilibrium science. The laws of thermodynamics apply to objects or systems in equilibrium with themselves and their surroundings. By definition, a system in equilibrium is not likely to change. However, we are generally interested in how systems change as thermal energy is converted to and from other forms of energy. This presents a bit of a dilemma in that the fundamental laws are only good for a system in equilibrium, and the parameters we want to predict are a result of thermal energy changes in the system. To get around this dilemma, we define what is called a quasi-equilibrium process. A quasiequilibrium process is one that moves from one system state to another so slowly and so incrementally that it looks like a series of equilibrium states. This is a concept that classical thermodynamics had a great deal of difficulty clarifying and quantifying. Basically, a process was a quasi-equilibrium process if the laws of equilibrium thermodynamics could characterize it. This is sort of a circular definition, but once again, we will find that the atomistic view allows us to make some predictions and quantifications that identify a quasi-equilibrium process. Quasiequilibrium processes can occur very rapidly on timescales typical of human observation. For example, the expansion of the hot gases out the nozzle of a rocket engine can be well described as a quasi-equilibrium process with classical thermodynamics.

1.5 Open and Closed Systems

In the transfer and conversion of thermal energy, we will be interested in separating the entire universe into a system and its environment. We will mainly be interested in the energy transfers and conversions that go on within the system, but in many cases, we will need to consider its interactions with the rest of the world or its environment. Systems that consist of a *fixed amount of mass* that is contained within fixed boundaries are called closed systems. Systems that pass the mass back and forth to the environment will be called *open systems*. Both *open* and *closed systems* allow energy to flow across their borders, but the flow of mass determines whether they are open or closed systems. Open systems will also carry energy across their borders with the mass as it moves. Consider the simple compressed gas in the piston below as a *closed* system (Fig. [1.2\)](#page-26-0).

In analyzing the closed system, we will be concerned about the changes in the internal energy of the compressed gas as it interacts with its environment and the transfers of mechanical and thermal energies across its boundary.

In analyzing open systems, the concept of a *control volume* comes into play. The control volume is the boundary for the open system where the energy changes that

Fig. 1.2 A closed system

Fig. 1.3 An open system

we are interested in take place. The thing separates the open system from its environment. Consider the following open system where we have now allowed mass to flow in and out of the piston of our closed system above (Fig. 1.3).

The *control volume* looks a lot like our system boundary from before, and it is. The only difference is that we now allow mass to flow in and out of our control volume. Thermal and mechanical energy can still flow across the boundary or in and out of the control volume. The mass flowing in and out can also carry energy with it either way.

1.6 System Properties

In order to characterize a system, we will have to identify its properties. Initially there are three main properties that we will be concerned with—density, pressure, and temperature—all of which are intensive variables. We will use intensive properties to characterize the equilibrium states of a system. Systems will be

composed of pure substances and mixtures of pure substances. A pure substance is a material that consists of only one type of atom or one type of molecule. A pure substance can exist in multiple phases. Normally the phases of concern will be gas, liquid, and solid, though for many pure substances, there can be several solid phases. Water is an example of a pure substance that can readily be observed in any of its three phases.

A solid phase is typically characterized as having a fixed volume and fixed shape. A solid is rigid and incompressible. A liquid has a fixed volume but no fixed shape. It deforms to fit the shape of the container that is in it. It is not rigid but is still relatively incompressible. A gas has no fixed shape and no fixed volume. It expands to fit the container that is in it. To characterize a system composed of one or more pure components and one or more phases, we will need to specify the correct number of intensive variables required to define a state. Gibbs Phase Rule named after J. Willard Gibbs who first derived it gives the correct number of intensive variables required to completely define an equilibrium state in a mixture of pure substances. It is

$$
V = C - P + 2 \tag{1.3}
$$

 $V =$ Number of variables required to define an equilibrium state

 $C =$ The number of pure components (substances) present

 $P =$ The number of phases present

So for pure steam at sea level and above $100\,^{\circ}\text{C}$, we have 1 component and 1 phase, so the number of variables required to specify an equilibrium state is 2, typically temperature and pressure. However, temperature and density would also work. If we have a mixture of steam and liquid water in the system, we have 1 component and 2 phases, so only one variable is required to specify the state, either pressure or temperature would work. If we have a mixture like air that is composed of oxygen, nitrogen, and argon, we have 3 components and 3 phases (the gas phase for each component), we are back to requiring 2 variables. As we progress, we will introduce additional intensive variables that can be used to characterize the equilibrium states of a system in addition to density, pressure, and temperature.

1.6.1 Density

Density is defined as the mass per unit volume. The standard SI unit is kilograms per cubic meter (kg/m³). The standard English unit is pound mass per cubic foot (lbm/ft³). If the mass per unit volume is not constant in a system, it can be defined at a point by a suitable limiting process that converges for engineering purposes long before we get to the atomistic level. The inverse of density is specific volume. Specific volume is an intensive variable, whereas volume is an extensive variable. The standard unit for specific volume in the SI system is cubic meters per kilogram (m^3/kg) . The standard unit in the English system is cubic feet per pound mass (ft^3/lbm) .

1.6.2 Pressure

Pressure is defined as force per unit area. The standard unit for pressure in the SI system is the Newton per square meter or pascal (Pa). This unit is fairly small for most engineering problems, so pressures are more commonly expressed in kilopascals (kPa) or megapascals (MPa). The standard unit in the English system really does not exist. The most common unit is pounds force per square inch (psi). However, many other units exist and the appropriate conversion factors are provided in the Appendix.

Pressure as an intensive variable is constant in a closed system. It really is only relevant in liquid or gaseous systems. The force per unit area acts equally in all directions and on all surfaces for these phases. It acts normal to all surfaces that contain or exclude the fluid. (The term fluid includes both gases and liquids). The same pressure is transmitted throughout the entire volume of liquid or gas at equilibrium (Pascal's law). This allows the amplification of force by a hydraulic piston. Consider the system in the following Figure. In Fig. 1.4, the force on the piston at B is greater than the force on the piston at A because the pressure on both is the same and the area of piston B is much larger.

In a gravity field, the pressure in a gas or liquid increases with the height of a column of the fluid. For instance, in a tube containing a liquid held vertically, the weight of all of the liquid above a point in the tube is pressing down on the liquid at that point. Consider Fig. 1.5, then:

Fig. 1.6 Pressure measurement with manometers

$$
dp = \rho g dh
$$

$$
p(0) = P(H) + \int_{0}^{H} \rho g dh
$$
 (1.4)

Thus, the pressure at the bottom of the container is equal to the pressure on the top of the fluid in the container plus the integral of the weight of the fluid per unit area in the container.

This raises an interesting concept. Often it will be important to distinguish between absolute pressure and gage pressure. The preceding equation calculates the absolute pressure. The gage pressure is simply the pressure exerted by the weight of the column without the external pressure on the top surface of the liquid. It is certainly possible to have a negative gage pressure, but not possible to have a negative absolute pressure. A vacuum pressure occurs when the absolute pressure in a system is less than the pressure in the environment surrounding the system.

Using the setup in Fig. 1.6, a very common way of measuring pressure is an instrument called a manometer. A manometer works by measuring the difference in height of a fluid in contact with two different pressures. A manometer can measure absolute pressure by filling a closed end tube with the liquid and then inverting it into a reservoir of liquid that is open to the pressure that is to be measured. Manometers can also measure a vacuum gage pressure. Consider Fig. 1.6.

The tall tubes on the right in each system are open to the atmosphere. System A is operating at a small negative pressure, or vacuum, relative to the atmosphere. System B is operating at a positive pressure relative to the atmosphere. The magnitude of the pressure in each case can be calculated by measuring the height difference between the fluids in the two sides of the U-tube and calculating its weight per unit area. This is the difference in the pressures inside the Systems A or B and the atmospheric pressure pushing down on the open columns on the right.

1.6.3 Temperature

The other intensive variable to be considered at this point is the temperature. Most everyone is familiar with temperature as a measure of coldness or hotness of a substance. As we continue our study of thermodynamics, we will greatly refine our