Development of a parametric analysis microcomputer model for evaluating the thermodynamic performance of a reciprocating Brayton cycle engine

Thomas J. White
Portland State University

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A microcomputer model has been developed which predicts the thermodynamic performance of a PACE engine. This engine operates, in principle, similar to the gas turbine engine, except it has
reciprocating piston compressor and expander components rather than aerodynamic blades. In this thesis, the PACE engine is modeled as an open Brayton cycle without regeneration.

The model incorporates all important irreversibilities found in piston devices including: heat transfer, pressure losses, mass loss and recirculation, and mechanical friction. There are thirty-eight input parameters. Key independent operating parameters are maximum combustor temperature, compressor RPM, and pressure ratio. Other input parameters are grouped into design characteristics of both the compressor and expander, operation parameters which characterize the irreversibilities, and properties of the working fluid.

In this thesis, applicable data from research on IC engines have been adapted to PACE engine designs. Data from studies on heat transfer, friction, and pressure losses, in particular, have been used. Certain parameters which define operation and design characteristics appear to influence PACE engine performance very strongly. Some of the more critical parameters, notably friction and heat transfer coefficients, must be determined experimentally if accurate model results are to be expected. Pressure ratio, compressor RPM, and maximum combustor temperature, the independent operating parameters, also have a dramatic effect on engine performance. Other design or operating characteristics and working fluid properties are not controlled independently. These are dictated by the engine physical design configuration and operation, ambient conditions, and choice of fuel.
Both a variable speed drive (VSD) coupling between the compressor and expander and a variable volume expander (VVE) are design options which allow the expander to reach full expansion. The VSD design was exercised extensively in the analyses and a complete sensitivity analysis was performed on all the input parameters. The emphasis in using the model is on relative comparisons rather than absolute accuracy in results. The reason for this is simple: a model is only as good as its least accurate assumption. Many of the assumptions and input data for the PACE model cannot be verified without additional experiments.

The PACE engine microcomputer model has demonstrated itself to be very useful for evaluating the effects of different input parameters on three engine performance indices: efficiency, net specific work, and power density. The model is interactive and sensitivity analysis is easily performed. The model is a very powerful tool for comparing the influences of different parameters and analyzing PACE components and engine design configurations. This work is the first step in developing a comprehensive model to analyze the thermodynamic performance of the PACE engine as a complete system.
DEVELOPMENT OF A PARAMETRIC ANALYSIS MICROCOMPUTER MODEL
FOR EVALUATING THE THERMODYNAMIC PERFORMANCE OF A
RECIPROCATING BRAYTON CYCLE ENGINE

by

THOMAS JOSEPH WHITE

A thesis submitted in partial fulfillment of the requirements for the degree of

MASTER OF SCIENCE
in
MECHANICAL ENGINEERING

Portland State University
November 1987
TO THE OFFICE OF GRADUATE STUDIES AND RESEARCH:

The members of the Committee approve the thesis of Thomas J. White presented November 20, 1987.

George A. Tsongas, Chairman

C. William Savery

Larry D. Simmons

B. Kent Hall

APPROVED:

C. William Savery, Head, Department of Mechanical Engineering

Bernard Ross, Vice-Provost of Graduate Studies and Research
ACKNOWLEDGMENTS

This work is a continuation of the analytic studies undertaken in the last few years by Dr. Reiner Decher at the Department of Aeronautics and Astronautics of the University of Washington. The PACE engine (Piston All-Fuels Ceramic Engine) has been under development since the late 1970's, and was originally conceived by Mr. Al Albert of Combustion Research Technology, Inc. of Seattle, Washington.

I began this thesis two years ago. The challenge of trying to model the novel PACE design coincided naturally with my interests in engines, thermodynamics, and computer modeling—all of which I have emphasized in my graduate studies curriculum and tapped extensively as resources for this project. Al Albert offered a grant to cover my tuition and other expenses, and the work began. I am grateful for Al's financial support and his patience in waiting two years for the final results.

I also owe a debt of gratitude to Zelimir Dobovišek, visiting professor from the University of Maribor in Yugoslavia, for sparking my interest in engines during the summer of 1984 when I took the course he taught on internal combustion engines at Portland State University.

Being a part-time graduate student, I have not always found time to put a concerted effort on this project with all the competing priorities in my life. Over the time I have worked on this project I have also worked full time as a project engineer at the Bonneville Power
Administration. To complicate my life even further, my wife and I have shared the joys and responsibilities of raising two very active preschool boys.

After all this time, it has been very satisfying to complete this work and see it extended beyond its original scope. Last summer, Larry Martin, another mechanical engineering graduate student at PSU, took my basic Apple IIe software program and translated it to an IBM PC version, and greatly improved the model. His enhancements have made the model more accessible and, most importantly, he has made interactive graphics output possible.

I wish to thank all the members of my thesis committee: Dr. Bill Savery, Department Head, for his continued support and encouragement over the several years I have been a graduate student at PSU; Dr. Larry Simmons, Professor of Mechanical Engineering at the University of Portland, for helping me to keep a balanced perspective and for his advice and participation in this project; Dr. Reiner Decher, from the University of Washington, for helping lay the groundwork for this project and providing guidance from time to time, especially early on when it was difficult getting started; and last but not least, Dr. George Tsongas, my adviser, for his willingness to work with me, any time, for as long as it took, to get a good quality job done. I am especially grateful for George's encouragement and support during this project and for the confidence in me he has shown.

Lastly, there are those who have supported and encouraged me, but have had no direct involvement in this project: my wife, Maureen, and my two children, Zack and Adam. There have been many nights and weekends I
have had to be a student instead of a husband and a father. I will always be grateful for the sacrifices my family has made on my behalf. In particular, I am indebted to Maureen for her patience and her faith in me. This has been the greatest encouragement of all.
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<tr>
<td>$A_i$</td>
<td>piston/valve area ratio, inlet</td>
<td>[dimensionless]</td>
</tr>
<tr>
<td>$A_e$</td>
<td>piston/valve area ratio, exit</td>
<td>[dimensionless]</td>
</tr>
<tr>
<td>$A_p$</td>
<td>area of piston face</td>
<td>[ft$^2$]</td>
</tr>
<tr>
<td>$A_v$</td>
<td>average valve opening area</td>
<td>[ft$^2$]</td>
</tr>
<tr>
<td>$a_s$</td>
<td>sonic velocity</td>
<td>[ft/sec]</td>
</tr>
<tr>
<td>$B$</td>
<td>number of cycles per revolution</td>
<td>[rev$^{-1}$]</td>
</tr>
<tr>
<td>$b$</td>
<td>bore</td>
<td>[in]</td>
</tr>
<tr>
<td>$C_i$</td>
<td>mean inlet flow coefficient</td>
<td>[dimensionless]</td>
</tr>
<tr>
<td>$C_e$</td>
<td>mean exit flow coefficient</td>
<td>[dimensionless]</td>
</tr>
<tr>
<td>c.v.</td>
<td>clearance volume (percent of stroke volume)</td>
<td>[%]</td>
</tr>
<tr>
<td>$c_p$</td>
<td>constant volume specific heat</td>
<td>[BTU/lb$_m$-°F]</td>
</tr>
<tr>
<td>$c_v$</td>
<td>constant pressure specific heat</td>
<td>[BTU/lb$_m$-°F]</td>
</tr>
<tr>
<td>$e_E$</td>
<td>expander component efficiency</td>
<td>[dimensionless]</td>
</tr>
<tr>
<td>$e_C$</td>
<td>compressor component efficiency</td>
<td>[dimensionless]</td>
</tr>
<tr>
<td>$e_H$</td>
<td>combustion efficiency (heat input efficiency)</td>
<td>[dimensionless]</td>
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<tr>
<td>$e_t$</td>
<td>engine thermal efficiency</td>
<td>[dimensionless]</td>
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<tr>
<td>$e_v$</td>
<td>volumetric efficiency (compressor)</td>
<td>[dimensionless]</td>
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<tr>
<td>$f$</td>
<td>friction coefficient</td>
<td>[fmep/(ft/s)]</td>
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<tr>
<td>fmep</td>
<td>friction mean effective pressure</td>
<td>[psi]</td>
</tr>
<tr>
<td>$G$</td>
<td>working fluid mass flow per cross section area</td>
<td>[lb$_m$/sec-ft$^2$]</td>
</tr>
<tr>
<td>$g_c$</td>
<td>conversion factor (32.2)</td>
<td>[lb$_m$-ft/sec$^2$-lb$_f$]</td>
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<tr>
<td>$h_e$</td>
<td>overall effective heat transfer coefficient</td>
<td>[BTU/sec-ft$^2$-°F]</td>
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<th>Description</th>
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<tr>
<td>J</td>
<td>conversion factor (778 ft-lbf/BTU)</td>
<td>[ft-lbf/BTU]</td>
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<tr>
<td>K</td>
<td>overall heat transfer coefficient</td>
<td>[dimensionless]</td>
</tr>
<tr>
<td>k</td>
<td>gas conductivity (standard air values)</td>
<td>[BTU/sec-ft-°F]</td>
</tr>
<tr>
<td>M</td>
<td>mass</td>
<td>[lbm]</td>
</tr>
<tr>
<td>( \dot{m} )</td>
<td>mass flow rate</td>
<td>[lbm/sec]</td>
</tr>
<tr>
<td>( \dot{m}_f )</td>
<td>fuel mass flow rate</td>
<td>[lbm/sec]</td>
</tr>
<tr>
<td>N</td>
<td>number of cylinders</td>
<td>[none]</td>
</tr>
<tr>
<td>n</td>
<td>modified polytropic exponent (for mass loss)</td>
<td>[dimensionless]</td>
</tr>
<tr>
<td>P</td>
<td>power density (based on expander displacement)</td>
<td>[HP/in³]</td>
</tr>
<tr>
<td>Pr</td>
<td>Prandtl number</td>
<td>[dimensionless]</td>
</tr>
<tr>
<td>p</td>
<td>pressure</td>
<td>[psia]</td>
</tr>
<tr>
<td>( \bar{p} )</td>
<td>mean cycle pressure</td>
<td>[psia]</td>
</tr>
<tr>
<td>( p^* )</td>
<td>critical pressure</td>
<td>[psia]</td>
</tr>
<tr>
<td>( P_r )</td>
<td>reservoir pressure</td>
<td>[psia]</td>
</tr>
<tr>
<td>( Q_H )</td>
<td>heat input rate at the combustor (heater)</td>
<td>[BTU/sec]</td>
</tr>
<tr>
<td>( \dot{Q}_H )</td>
<td>heat content of the fuel</td>
<td>[BTU/sec]</td>
</tr>
<tr>
<td>( Q_C )</td>
<td>heat loss from the compressor</td>
<td>[BTU/sec]</td>
</tr>
<tr>
<td>( Q_E )</td>
<td>heat loss from the expander</td>
<td>[BTU/sec]</td>
</tr>
<tr>
<td>R</td>
<td>gas constant</td>
<td>[ft-lbf/lbm-°F]</td>
</tr>
<tr>
<td>Re</td>
<td>Reynolds number</td>
<td>[dimensionless]</td>
</tr>
<tr>
<td>( R_C )</td>
<td>pressure ratio, compressor operating parameter</td>
<td>[dimensionless]</td>
</tr>
<tr>
<td>RPM</td>
<td>revolutions per minute</td>
<td>[min⁻¹]</td>
</tr>
<tr>
<td>r</td>
<td>a volume ratio, see EQ. 3.4</td>
<td>[dimensionless]</td>
</tr>
<tr>
<td>s</td>
<td>stroke</td>
<td>[in]</td>
</tr>
<tr>
<td>T</td>
<td>temperature</td>
<td>[°F]</td>
</tr>
<tr>
<td>( T_g )</td>
<td>mean effective gas temperature (for a cycle)</td>
<td>[°F]</td>
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\[ T_{\text{max}} \] maximum cycle temperature at combustor [°F]

\[ T_c \] mean coolant temperature [°F]

\[ u \] mean piston speed [ft/sec]

\[ V \] volume [ft^3]

\[ \text{VSD} \] variable speed drive coupling --

\[ \text{VVE} \] variable volume expander --

\[ V_{cv} \] clearance volume [ft^3]

\[ V_C \] swept volume, compressor [ft^3]

\[ V_E \] swept volume, expander [ft^3]

\[ V_e \] expanded volume, compressor residual gases [ft^3]

\[ V_I \] intake volume of the expander (same as \( V_I \)) [ft^3]

\[ V_x \] volume at the end of an isentropic process [ft^3]

\[ V_y \] volume reduced by mass loss [ft^3]

\[ v \] gas velocity through an orifice [ft/sec]

\[ W \] total work [ft-lbf]

\[ \dot{W} \] power [ft-lbf/sec]

\[ \dot{W}_f \] rate of friction work [ft-lbf]

\[ w \] net specific work [ft-lbf/lbm]

\[ Y \] mass loss fraction [dimensionless]

\[ y \] a pressure ratio, see EQ. 3.4 [dimensionless]

\[ Z \] Mach index [dimensionless]
SUBSCRIPTS

C, E, H refers to the compressor, expander, and combustor (heater)

' (prime) denotes adiabatic or post-combustion gas properties

1 and 2 refers to compressor and expander; determined by context

i and e inlet and exit

i and a ideal and actual

GREEK SYMBOLS

\( \alpha \) thermal diffusivity (see also EQ. 3.4)

\( \beta \) mass loss parameter (see EQ. 3.13)

\( \gamma \) ratio of specific heats, \( c_p/c_v \)

\( \delta P_1 \) pressure drop at compressor inlet (psia)

\( \delta P_2 \) pressure drop across the combustor (\%)

\( \varepsilon \) polytropic multiplier (see EQ 2.27)

\( \eta_a \) admission coefficient (expander)

\( \lambda \) mass loss factor exponent

\( \mu \) dynamic viscosity [lbf-sec/ft^2]

\( \rho \) density [lbm/ft^3]

\( \sigma \) \( (\gamma-1)/\gamma \)

\( \phi \) equivalence ratio, [dimensionless]
CHAPTER 1

INTRODUCTION

In recent years a novel engine, called the PACE, has been under development at a small R&D firm, Combustion Research Technology, Inc., in Seattle, Washington. PACE (originally called the Britalus) is an acronym for Piston All-Fuels Ceramic Engine. This engine is based on an open Brayton cycle. The design uses reciprocating piston components for compression and expansion (work output) rather than the rotating, aerodynamic airfoil blades used in axial compressors and turbines in the most common application of the Brayton cycle -- the gas turbine engine. Unlike conventional spark-ignition and Diesel internal combustion (IC) engines, the PACE separates compression, expansion, and combustion into three different components and does not have the temperature and pressure profiles seen within the cylinders of IC engines.

Compared to the gas turbine design, the PACE has several outstanding potential advantages. Piston components can be scaled over a very wide range, making the PACE much more versatile for small-scale power applications compared to turbomachinery which is limited to relatively higher scale power (upwards of 500 kW and beyond). PACE has a broader acceptance of different combustion fuels because the combustor can be isolated easily from the working fluid process stream to avoid contamination problems. Combustion can also be carefully controlled,
getting better burn efficiency while eliminating most pollutants. As for cost, the PACE could be much lower in cost than its IC cousins. Increased durability, and therefore, reliability and maintainability may be a benefit of reduced temperature and pressure stresses compared to IC engines.

With the prospect of incorporating ceramic liners into PACE cylinders, it may be possible for higher temperatures to be tolerated and thermal efficiency might be improved. The PACE does not have the same metallurgical temperature limits of conventional gas turbine systems because it does not use turbine blades. Higher pressure ratios than those possible with axial or centrifugal compressors will also improve efficiency. Part load characteristics are favorable because power is tied to mass flow rate which can be adjusted over a wide range of RPM without severe performance penalty.

However, there are certain disadvantages that a piston-style Brayton cycle engine suffers over its aerodynamic gas turbine analog. Friction losses associated with piston movement and flow losses at the entry and exit ports of the cylinders are two potentially significant penalties. But, the use of specially designed sleeve valves for both the expander and compressor will largely eliminate the loss of work availability from pressure losses typically experienced by IC engines with cam operated valves. Operating at relatively low engine RPM can reduce both pressure losses and friction irreversibilities which are primarily speed dependent.

The development of the PACE engine has reached a stage where a thorough analysis of the engine's performance capabilities, modeled as a
thermodynamic system, will be the most direct and economical means to
guide further advances in the development of this innovative power
technology. "Where do we go next?" can best be answered by evaluating
the range of operating parameters the PACE engine is likely to be
designed to work under. An investigation into aspects of engine design,
such as the effects of varying pressure ratios, different valve designs,
RPM, maximum temperature of the working fluid, friction losses, and
evaluation of heat transfer characteristics, can direct hardware
development and testing toward the most productive, optimum design
alternatives. This could easily save many hours of trial-and-error
testing in the laboratory and fabrication costs in the shop.

With this in mind, a computer model has been developed and tested
which is capable of performing the kind of parametric analyses
described. The availability, interactive facility, and computing power
of today's inexpensive microcomputers make this modeling approach a very
effective means to arrive at a more thorough understanding of the
capabilities and limitations of the PACE engine concept.

The end result is a software package which simulates the
performance of the PACE engine under a wide variety of possible
operating conditions. It also allows for easy interactive input and
rerunning of varying sets of engine design and operating parameters.
The algorithms are based on sound thermodynamic principles and empirical
data derived from experiments with IC engines. Once a preferred PACE
design configuration is determined, the software model can be used to
work toward an optimum design by looking at trade-offs and interactive
effects among various design and operating parameters.
Results of an extensive parametric and design analysis are presented in Chapter 5. Overall, the analysis points toward the need to investigate the friction and heat transfer characteristics of working PACE compressor and expander components to narrow the value range of the input data associated with these parameters. In addition, results indicate clearly the effect of valve design and operation on volumetric efficiency and pressure losses on the three key performance indices: net specific work, overall engine thermal efficiency, and power output. Actually, most of the ensuing analyses use power density, rather than power, as a performance index. Power density is just power divided by the volume displacement of the expander cylinders, and using this index is a way to normalize performance information. We turn now to a description of the PACE engine design and operation, then a summary of the approach used to develop the thermodynamic relationships, program the software, and complete the engine analysis.

1.1 Description of the PACE Engine

A diagram of the initial PACE design concept can be found in Fig. 1.1. Both the PACE compressor and expander components of the engine have a common design, but the expander operates in reverse fashion from the compressor. There are three key parts of the PACE design: a three-lobed cam, a rotor with six pistons, and a central manifold. As the rotor turns, each piston moves up and down within its respective cylinder in simple harmonic motion (i.e. displacement can be described by a sine function). In one revolution there are 18 induction
Fig. 1.1 -- PACE (Britalus) Compressor Design

Note the three-lobed stationary cam, the stationary interior manifold, and the rotor with pistons (after Decher [6]). Expander design is similar, but rotation is in opposite direction.
and discharge cycles -- three cycles per cylinder, times six cylinders. At any time during a revolution, there are always three pistons at the same phase of compression or expansion.

At the apex of a one of the cam lobes, a piston is at outer, or top, dead center (TDC), or at its maximum expansion (see also Fig. 1.2); a full compression/expansion cycle is equal to 60 degrees of revolution. At TDC the cylinder volume is at a minimum, and at bottom dead center (BDC) the piston has swept the full cylinder volume. Piston contact at the cam surface is by a roller bearing designed to maintain uniform pressure and a positive tangential rotational force. The central manifold channels allow for both induction and expulsion of the working fluid. The amount of mass flow entering the cylinder is controlled by the duration of exposure the cylinder port sees at the manifold-piston interface. Note that the intake or exhaust manifold openings can be advanced or retarded to change the compression/expansion profile of the cycle within the cylinder (see Fig. 1.2) by inducting more air or expelling air before the piston reaches BDC. By adjusting the intake and exhaust periods in this way, the pressure ratio in the expander or the compressor can be easily modified, and a great deal of control can be exerted over engine operation.

A second generation PACE compressor and expander design is now being emphasized, but it differs somewhat from the first design (the one shown in Fig. 1.1 has been dubbed 'PACE I'). The second design (PACE II) has a planetary gearing system rather than a cam casing. Rather than having the pistons turn with the rotor, the pistons remain stationary and the manifold rotates instead. This second generation
Fig. 1.2 -- Profile of PACE Compressor Process

Shows simple harmonic motion where "D" denotes design points for (1) admission, (2) beginning of compression, (3) end of compression, beginning of discharge. $\Theta$ is degrees of crank angle. PACE expander operates similarly (after Decher [6]).
design eliminates the piston forces due to angular and Coriolis accelerations but requires a more complex gearing arrangement to transmit the torque from the cylinders.

1.2 Thermodynamic Analysis

Analytic work completed to date on the PACE engine design concept has emphasized compressor and expander characteristics and modeling non-ideal, irreversible processes to determine certain performance capabilities such as specific work versus efficiency. This thesis integrates work already completed into a comprehensive system model and refines the equations that describe pressure losses, heat transfer, and friction irreversibilities of an operating PACE engine. Such a complete model helps provide answers to questions like "what effect does doubling the friction coefficient have on power output?" or "what is the trade-off between efficiency and power over a given performance range?" By combining the influences of all principal operating parameters into this model, a user can evaluate the effects of a set of operating conditions on certain performance indices such as efficiency, specific work, or power.

Fig. 1.3 is a schematic diagram of the engine design to be modeled, comprising the three basic components: the compressor (C), the combustor or heater (H), and the expander (E). Each irreversibility, and where it occurs, is designated by a two-letter code. The derived equations and thermodynamic relationships form the foundation for an engine model, and account for four sources of irreversibilities in the
Air Properties (pre-combustion) $\mu, \rho, \gamma, K, C_p, C_v, R$

Combustion Gas Properties (post-combustion) $\mu', \rho', \gamma', K', C'_p, C'_v, R'$

Fig. 1.3 -- PACE Engine Diagram with Irreversibilities

HT -- heat transfer
FR -- friction
PR -- pressure losses
MA -- mass loss and recirculation
compression, expansion, discharge, admission and heat addition processes of the PACE engine:

1. **Pressure losses**--PR:
   + entry and exit losses at the cylinder port/manifold interface of both the compressor and expander
   + duct losses into and out of combustor burner (or heater)
   + includes flow work necessary to induct or expel working fluid through valve openings

2. **Heat losses (non-adiabatic processes)**--HT:
   + heat transfer from the gas to the cylinder walls, both compressor and expander (high pressure gas temperature loss in the expander being the most important)
   + heat losses from the combustor, or combustion inefficiency

3. **Friction work losses**--FR:
   + work necessary to overcome mechanical friction in the compressor and in the expander (piston rings and valve/gear systems)

4. **Mass leakages and mass recirculation**--MA--:
   + compressor and expander -- recirculation of gases trapped in the clearance volume after discharge
   + compressor and expander -- effectiveness of piston and valve seals separating cylinder from manifold

In Chapter 2, relevant data and analysis from other authors is assessed as a basis for the PACE engine model. All of the irreversibilities are functions of two key parameters -- speed and pressure ratio. This may seem an over-simplification, but further analysis reveals the insight of this statement. Mass flow rates are dictated by RPM (speed) and so is friction. Heat losses are a direct function of temperature difference and mass flow rates as well as fluid density, which is a function of pressure. Pressure losses are a direct result of flow passage configuration (physical dimensions), mass flow
rate, and pressure differential. Mass leakage is also a function of pressure differential and inversely related to speed. Pressure differential, at any point in the Brayton cycle process, is a function of the compressor pressure ratio. Recall that the Brayton cycle is a constant pressure heat addition process, so the maximum pressure is the pressure at the end of compression. Any excess work or lost availability can be traced to these irreversibilities. Every important engine performance characteristic can therefore be analyzed as a function of RPM and compressor pressure ratio.

The irreversibilities account for all the excess work or loss of work availability as the working fluid progresses through the compressor, combustor, and expander. It is the inter-relationships among these non-ideal processes, under varying operating conditions, that give the PACE its unique performance characteristics. Because of the reciprocating design feature of the PACE, compared to, say, its gas turbine cousin, the PACE can be shown to be uniquely influenced by some irreversibilities more than others. Note that in gas turbines, or any aerodynamic device, there are significant flow losses due to momentum transfer and fluid friction. This is not the case in the PACE where the chief irreversibilities are mechanical friction, heat transfer, and pressure losses at the ports.

It is the purpose of this project to model these processes, as functions of appropriate input parameters, to help determine optimum design configurations and operating conditions. It is the model's capability to analyze non-ideal processes -- where the PACE engine's performance deviates from the ideal Brayton cycle -- that is the most
important feature of this model. The engine model is based on the several assumptions which are discussed in detail in Chapter 3. This chapter develops the analytic foundation, or methodology, used for the PACE model.

1.3 Software Program Design

The emphasis of the software development is the creation of a parametric analysis model capable of evaluating the performance of the PACE engine given any set of pre-defined operating conditions and parameters for a particular design configuration. This software is a tool for analyzing the PACE engine performance characteristics and optimizing design improvements.

Chapter 4 describes the design details of the PACE engine software model. Appendix B lists the model source code in Applesoft BASIC. Other details of the system software and hardware are provided in Section 4.2. The model is a basic structured program, with distinct input, analysis, and output modules.

The program has the flexibility to rerun its simulation once the user has had the opportunity to evaluate the output and decide whether certain parameters should be changed. With this parametric analysis feature, only those values the user wishes to modify need to be specified, leaving the rest of the input data intact.

However, certain input data are interdependent: a change in one parameter requires a corresponding change in another parameter. Even with large mainframe simulation models, a computer is limited in its
sophistication when trying to accommodate all combinations of inputs and to figure out which ones are interdependent. Only a certain set of combinations of input parameters will work. One way to handle this problem is to provide error messages during the simulation that indicate possible corrective measures a user might take to ensure interdependent parameters have been changed concurrently, making the input consistent. The PACE software model does this.

The calculations portion of the program consists primarily of determining pressure, temperature, and density (thermodynamic state points), and volumes and mass flow values which are essential for the engine performance analysis. The model does this by accommodating all non-ideal processes such as non-adiabatic heat addition, friction work, volumetric inefficiencies, and pressure and mass losses.

In testing this program there were two phases, commonly referred to as alpha and beta tests. Alpha phase is the stage of debugging and testing when the programmer runs the software thoroughly through its paces. The goal is to uncover any kind of bug or problem with the software to make sure it does what it was designed to do. The beta phase is conducted by users other than the software developer, by being tested extensively in applications where the software was designed to be used.

This software has the same limitations of any microcomputer model including relatively slow processing speed and restrictions which can be attributed to hardware. In particular, there are input/output (I/O) constraints, where the options to access disk, printer, or plotter, are limited. The model also has the inherent deficiencies associated with
the BASIC language. It lacks structured syntax and shell routines, has a slow interpreter, and its I/O features are considered primitive compared to other high level languages. However, subsequent improvements in the model may eliminate some of these limitations.

Corroboration, or validation, of the model with other similar results has turned out to be difficult. Because the model resolves the compressor and expander processes into four discrete parts it is not easily compared to the work already completed on the PACE, which tended to focus on other analytic problems. Furthermore, there are few similar engine designs to make comparisons against. Those that have been developed have empirical data which do not fit directly into this model's analytic framework. Model validation is described further in Section 4.5.

1.4 Parametric Analysis and PACE Engine Performance Characteristics

After the programming was completed and the software had been tested, a systematic engine design and parametric analysis was planned (see Table 5.1). In this last phase, the relevant input and output

* For the compressor, the four processes are admission, compression, discharge, and re-expansion of the clearance volume residual gases. For the expander, the order is reversed: intake, expansion, exhaust, and recompression of residual gases. Note that the induction and expulsion processes are referred to as admission/discharge for the compressor and intake/exhaust for the expander. This distinction in terms is arbitrary, but will help to keep the compressor processes separate from those of the expander.
parameters, and ranges of these parameters, to be used in the program were defined for the parametric analysis. The model emphasizes three key performance indices for evaluating engine performance: net specific work, efficiency, and power density.

Results of these analyses are presented in Fig. 5.1 to 5.12 in Chapter 5. Overall, these results can only be useful for comparative analysis without better empirical data for friction and heat loss factors. The graphs represent a reasonable range for all the parameters and show trends, peak values, or other relationships among the design and operating parameters analyzed. Specifically, the principal output information is a set of what may be called compressor/expander "maps" for the engine (see Fig. 5.2). Ultimately, the objective of this analysis is to focus on the most critical design parameters, illuminating a path toward the most productive development work.

After the engine map was generated, further analysis was undertaken to determine which parameters have the greatest influence on optimum engine performance. A detailed optimization study is not within the scope of this project, primarily because an exhaustive set of comparative parametric runs and sensitivity analyses would need to be done to complete the work. Moreover, the model does not determine a mathematical optimum design. But it does lend itself to varying design configurations toward achieving specific design objectives. Again, the focus of this project has been to develop a system model of a PACE design and evaluate the engine's performance characteristics.
1.5 Other Considerations and Model Limitations

In this analysis, the emphasis is on the performance of the PACE compressor and expander. Consequently, details of combustor design and combustion processes are lumped into broad parameters to simulate heat loss, pressure loss, and fuel conversion efficiency for the heat addition process. Combustor pressure and heat losses can be minimized by a variety of burner designs, and it is not within the scope of this project to focus on this particular problem.

Furthermore, in reporting the performance characteristics and analysis results of this project, only brief comparisons to other internal combustion engine characteristics (such as the Diesel or the gas turbine engines) are made, where appropriate. It is not within the scope of this project to provide a detailed comparative evaluation of the PACE design versus other engines.

One could use the parametric analysis mode of the PACE software program to determine the relative effects of changing certain components or parameters; peak values, trends, and interrelated effects can all be discerned by using this model. However, there is virtually an unlimited set of possibilities for variations in system configuration and design values. As noted earlier, this software is not able to determine which component or component variables should be 'optimized'.

1.6 Thesis Development and Chapter Summary

The approach taken in establishing the thesis methodology was to first review the previous work in the literature to gather relevant
information, then to adapt this information and develop the algorithms and equations for the model. The first part is presented in Chapter 2, the second in Chapter 3. Chapter 2 describes how others have dealt with thermodynamic cycle irreversibilities, but stops short of telling how the information is used in the model. Chapter 3 goes beyond the foundations in Chapter 2 and actually defines the equations used in the PACE software model. Chapter 3 lists all model assumptions, and completes the First Law of Thermodynamics analyses for defining compressor and expander component efficiencies and engine net specific work, power, and efficiency.

Chapter 4 identifies all the input data required for the algorithms and divides these input parameters into five groups, with a total of 38 parameters. The five groups are: compressor design characteristics, expander design characteristics, operation characteristics, working fluid properties, and operating parameters. These inputs or parameters are described further in Chapter 5. Chapter 5 also develops five uses of the model: preliminary engine design, creation of engine performance "maps", sensitivity analysis, parametric analysis, and analysis of parameter interactive effects.

Finally, Chapters 6 and 7 summarize the key features and limitations of the model and propose follow on work to improve the model, enhance the software, and complete more extensive analysis.
CHAPTER 2

THERMODYNAMIC FOUNDATIONS FOR THE PACE ENGINE

Modeling the performance of the PACE engine requires that appropriate relationships which account for the irreversibilities of the PACE processes be derived first. In searching for ways to define a mathematical model which represents an operating PACE engine, we find there are three sources which can be tapped: work already done on the PACE engine itself; results reported in the literature on similar reciprocating compressor and expander devices; and finally, work done on IC engines which may be applicable to the PACE engine. This chapter reviews the literature, while the next chapter establishes the equations and algorithms based on the information developed in this chapter.

Most of the analytic work to date on the PACE engine has been conducted by Reiner Decher of the University of Washington. Decher's studies are ongoing, and this thesis work is an extension of his efforts. As for similar engines, the literature holds at least two designs which incorporate reciprocating pistons for both compressor and expander components of a Brayton cycle engine. One engine, called the valved hot-gas engine (VHGE), was built and tested at the Massachusetts Institute of Technology [1, 2].

*Numbers in brackets refer to references cited at the end of this report.
Another preliminary engine design, referred to as the reciprocating internal combustion engine with constant pressure combustion (RIC-CPC), originates from Mechanical Technology, Inc. [3]. A study by Rosa [4] of the University of Montana has tied these designs together along with other literature sources into a comprehensive framework for analyzing a piston-component Brayton cycle engine. These engine designs are discussed in more detail in subsequent sections.

There are other piston engines with characteristics similar to the PACE. The Ericsson and Stirling engines, for example, differ from the PACE Brayton cycle design primarily in heat addition, which is at constant volume for both of these engines rather than at constant pressure. While the Stirling design has a closed gas system with both a heat source and a heat sink, the Ericsson is a simple open system. Like the PACE, neither the Ericsson or the Stirling employs internal piston combustion. Heat is supplied external to the cylinder.

Another novel piston engine design, the GeRace, was reported recently in the literature [5]. This engine has opposing pistons in one long cylinder, with the space in between the two pistons used for combustion. The variation in both cylinder volumes over time depends on the cam design. The cylinders, mounted axially, ride on opposite fly-wheel cams much like the rods holding the horses ride the rolling floor of a merry-go-round. This engine concept has promise compared to conventional IC engine design because combustion can be controlled better. Cam adjustments, which are independent for both sets of opposing pistons, make part load control very simple. The design also
has the advantage of sliding valves, and can use compression braking to slow the engine RPM.

Finally, the literature abounds in detailed information on heat transfer, valve losses, friction, volumetric efficiency, and other topics pertaining to the analysis of IC engine performance. Out of necessity, some of this information has been adapted in this thesis to try to model the PACE engine's unique design and operating characteristics because good empirical data, which would apply to the PACE, simply does not exist.

2.1 Summary of PACE Engine Work Completed to Date

In 1970, Combustion Research Technology, Inc. (CRTi) of Seattle, Washington, initiated the design and development of the PACE concept, eventually patenting the design in 1982. The PACE was formerly called the Britalus, which is an abbreviated name for Britain-Italy-United States, the home countries of the original engineers who worked on the engine.

Private funding has been used to construct and test a working prototype PACE I compressor. The compressor has run for over 500 hours without significant problems. Preliminary analysis indicates operational adiabatic efficiencies of up to 80% should be possible. Meanwhile, a modified design PACE II compressor prototype has just recently been built and is being tested.

A series of technical papers on a number of distinct performance aspects of the PACE engine design and operation have been completed by
Reiner Decher of the Department of Aeronautics and Astronautics at the University of Washington [6 - 11]. These analytic studies, as well as the prototype testing of the PACE I compressor completed to date, suggest that the PACE concept has considerable merit and warrants further development.

Decher's analytic modeling undertaken so far has dealt with four main topics:

1. Initial technical presentation [6, 7];
2. Part load performance control and optimization [8, 9];
3. Friction and power scaling characteristics [10];
4. Flow losses at the intake and exhaust ports [11];

In his first papers [6, 7], Decher introduces the PACE engine concept and discusses the problem of power output control. An important operating characteristic of displacement components, such as pistons, is that they process volumes of a working fluid. Also, in steady flow, the principle of mass conservation must be satisfied as the fluid is processed through the working components of an engine like the PACE. The expander must accommodate the same mass flow as the compressor delivers. But the density of the working fluid is drastically reduced because of the heat added during combustion. If the expander rotates at the same RPM as the compressor, and if both components have the same number of cylinders, then the expander cylinder must have a much larger displacement, or swept volume, than the compressor.

A simple means to control pressure ratio in the compressor of the PACE I engine is through variable timing, or shifting the exposure duration between the cylinder port and the manifold opening [8]. This scheme is particularly effective for part load control because power
output depends directly on pressure ratio. Decher shows how variable pressure ratio can be easily implemented. Also, his analysis describes how efficient part load operation necessarily involves a reduction in peak specific power. This can be accomplished through selection of the proper ratio of expander-to-compressor displacement.

Next, the question of obtaining good part load performance while maintaining high specific power arises. Decher also deals with this [3, 4]. There are many control options; several possibilities are discussed and graphed on T-s diagrams. Operating at other than the design pressure ratio will result in over or under expansion of the expander (see Fig. 2.1). Employing a variable speed drive (VSD) coupling between the expander and the compressor, or having a variable volume expander (VVE), are two ways to get around this problem. This strategy also allows for off-design, or part load, operation without excess losses from blowdown (the high temperature, high pressure gas which is exhausted from the expander well above ambient conditions).

Friction losses incurred by piston motion against cylinder walls are unavoidable but can be minimized by low RPM. Decher [10] discusses this problem at some length. He notes that low RPM also lowers the mass flow rate which diminishes specific work. Here is a classic trade-off between efficiency and specific work. Nevertheless, compared to the gas turbine engine, the possibilities of using higher temperatures with ceramic components may compensate for this disadvantage, and higher power ratings may be achieved at much lower RPM's. Also, since combustion does not take place in the cylinder, as with the Diesel and
Fig. 2.1 -- Over- and Under-Expansion in a PACE Expander
other IC engines, the concern over pulsed exposure to temperature extremes is also eliminated in the PACE design.

Dimensional scaling considerations are also reviewed in this paper. Unlike the gas turbine engine, where efficient operation is limited to large-scale power levels (usually more than 500 kW), many of the important performance characteristics of the PACE engine, such as specific power and efficiency, are scale-independent. The direct implication of this principle is that the PACE engine could prove attractive for relatively small-scale applications. However, the bore/stroke ratio (b/s) is the one scale factor which does influence heat transfer and friction, as will be explained later.

All displacement engines have a means for transferring a fresh charge of the working fluid efficiently into and out of the cylinder. In the PACE engine design, this is accomplished by periodic exposure of the cylinder port to either the high pressure or low pressure duct of the central manifold. The duration of opening, shape, and size of ports on both sides of this gas exchange interface have a profound influence on the pressure loss component of the engine's performance, affecting the overall efficiency of the engine's operation. In another publication, Decher [11] derives a key parameter, M, which describes this influence. It is a Mach-number like index which includes relative port size and pressure difference between the cylinder and the manifold. His analysis shows that the most significant pressure loss processes are at compressor discharge and at expander admission. (Note: In this thesis, Z is used as the Mach index, because it is consistent with the
symbols used by Taylor [12] and avoids the association of M with mass or mass flow).

Decher translates this pressure loss into an adiabatic efficiency for the compressor and expander work components, then derives a volumetric efficiency expression for the expander. For realistic values of the Mach index, these efficiencies are found to be high enough that the flow losses due to compressor discharge and expander admission are unimportant compared to piston friction losses.

Further work by Decher [13] is now being extended into aspects of heat transfer and combustor design, as well as expander characteristics, to complete the analytic framework for the design of the PACE engine and to aggregate the results of all previous analyses. Design, fabrication, and testing of an expander is planned as part of the comprehensive development work for the PACE engine. In the future, test results from these experiments will provide input data for the system computer model. It should be emphasized that while significant progress has been made toward development of the PACE engine—particularly design analysis—no comprehensive system model of the complete engine has yet been devised. Undertaking the development of such a software model, and then using it to explore future avenues of engine development, is the objective of this study.

2.2 Reciprocating Compressor and Expander Design

In principle, reciprocating compressors are very much like the PACE. The unique features of the PACE lie in its valve or port design
around a central manifold. This aspect alone should markedly increase volumetric efficiency and limit pressure losses. Without poppet valve cams, mechanical losses can also be minimized. There is a breadth of literature on reciprocating compressor design and operation [14 - 16]. However, there is almost nothing in the literature which gives an analytic foundation for piston expanders. The most common application of the piston expander is the locomotive steam engine drive. However, what is available on steam engine pistons tends to be mainly descriptive.

Compressors, on the other hand, are treated more comprehensively and more analytically. The literature clearly defines key operating and design characteristics of compressors, notably adiabatic efficiency and volumetric efficiency.

2.2.1 Reciprocating IC Engine with Constant Pressure Combustion (Warren and Bjerklie, 1969)

Warren and Bjerklie [3] of Mechanical Technology, Inc. proposed modifying a 450 cu.in. V-8 engine to operate similar to the PACE engine. Half the cylinders would be used for compression, the other half for expansion. The emphasis of their study was mainly on the advantages in the combustion process, with very little discussion regarding the other aspects of engine operation. The authors acknowledge the blowdown losses which result in lack of full expansion of the expander, which is understandable since all cylinders, both compression and expansion, have the same displacement volume. However, the authors suggest that this
engine, with regeneration, can match efficiencies of comparable IC engine designs. The authors also note that higher, consistent temperatures and compression ratios make this design very attractive. Although a sophisticated main-frame computer model was used to generate performance curves, details of friction, pressure losses, and heat transfer were not discussed, at least not enough to adapt algorithms for the PACE modeling work.

2.2.2 Valved Hot-Gas Engine (Lee and Smith, 1978)

An actual engine design of a reciprocating Brayton cycle engine, like the PACE, was reported initially by Lee and Fryer [1] in 1973, and, later, more developed by Lee and Smith [2]. Work on this engine began at the Cryogenic Laboratory of the Massachusetts Institute of Technology. This valved hot-gas engine (VHGE) is a closed-loop Brayton cycle design with regeneration, employing helium as the working fluid. The authors discuss both analytic and prototype test data to establish the capabilities and potential of the reciprocating Brayton cycle design. Initial analysis indicates efficiencies to be only about 1/2 to 2/3 those predicted. Key losses are attributed primarily to cyclic heat transfer, and some to mass leakage. Pressure losses and friction are not developed in detail. The problem of heat transfer is covered more appropriately in a subsequent part of this chapter.

The authors address the possibility of using ceramic materials to accommodate higher temperatures. However, there is a caution to consider strength, creep, cost, and weight compared to metal materials.
Ceramic coatings are offered as an alternative to a complete substitution of metal parts.

2.2.3 A Closed Brayton Cycle Piston Engine (Rosa, 1981)

Perhaps the most relevant study of a Brayton cycle, reciprocating engine design is the most recent, presented by Rosa [4]. His paper establishes a firm theoretical basis for treating friction, pressure losses, and heat transfer, based primarily on data from Taylor [12], while adapting the work of the other authors mentioned in the two previous sections. Rosa's analysis suggests that compressor and expander adiabatic efficiencies can reach upwards of 90%, while operating at average pressures of about one third of the peak pressures experienced in comparable IC engines. By constraining his analysis to a limited number of assumptions and operating conditions, Rosa suggests heat transfer in the expander (the main heat loss) can be calculated simply as a function of the inlet pressure and the piston speed. However, his heat transfer analysis is not general enough to accommodate a broad range of expander designs. More details of Rosa's treatment of friction and pressure losses are given in appropriate sections below.

2.3 Pressure Losses, Valve Design, and the Mach Index

Reciprocating pistons require valve and port arrangements to admit and expel gases in processing volumes of the working fluid. In IC engines, the work required to overcome the flow resistance of valve or port openings is called pumping work, experienced during both the intake
and exhaust strokes. Aerodynamic components, or rotating compressors and turbines, on the other hand, incur pressure losses due more to momentum transfer irreversibilities than pressure drops across openings. In reciprocating devices, flow resistance is responsible for a significant loss in work availability. Excess work is required to overcome this resistance.

Three aspects contribute to establishing a foundation for analyzing the pressure drops of port openings: valve design, valve operation, and average piston speed. Taylor develops each of these topics in great detail, citing ample evidence from the literature to derive an important parameter described here, the Mach index.

By definition, the Mach index (or Mach number) is the ratio of actual flow velocity to sonic velocity. At a Mach index of unity the flow regime reaches the maximum flow rate possible for a compressible fluid. Fluid theory predicts that subsonic fluid flow becomes limited to an absolute maximum flow at the critical pressure ratio, defined as follows:

\[
p^* / p_r = \left[ \frac{2}{V + 1} \right] \frac{Y}{Y - 1}
\]  \[2.1\]

where \( p^* \) is the critical pressure, \( p_r \) is the reservoir pressure and \( Y \) is the ratio of specific heats.

For air, with \( Y \) equal 1.4, the critical pressure ratio is 0.5283. In other words, if the reservoir pressure is more than about two times the back pressure, flow velocity will be constricted to a rate no higher than sonic velocity. This is called choked, or critical, flow. In IC engines, because cylinder and ambient pressures are very close at
intake, choked flow is not an important design consideration. But in the PACE, the expander inlet pressure is very much higher than the expander exhaust pressure. The ratio of the expander inlet pressure to ambient is, of course, very close to the design pressure ratio, $R_C$. Realistically, residual gas pressure should be recompressed equal to the inlet pressure in the expander to minimize pressure shock effects and the resultant pressure loss penalty. This can be accomplished by recompressing a portion of the residual exhaust gases near the end of the expander exhaust stroke. The idea here is to keep local velocities low enough (relative to the speed of sound) through ports and valve openings to minimize pressure losses.

Preliminary analysis suggests that the loss of availability resulting from sonic effects at the expander inlet may be less than the extra work necessary to recompress the residual exhaust gases. This point needs to be verified and warrants further study.

In a piston-cylinder arrangement, any constriction tends to compress the flow trying to exit; likewise, a piston trying to draw flow into an empty cylinder creates a relative vacuum. In the case of a cylinder discharging, the reservoir gas density increases, building a pressure differential across the valve opening. Similarly, the reservoir pressure in an inducting cylinder drops with the same effect: an increase of pressure differential.

If the fluid were incompressible, then the exit flow rate through the valve opening would be equal to the volume displaced by the piston times the average piston speed times the fluid density (see Fig. 2.2).
Fig. 2.2 — Diagram of Mass Flow Through a Port

Cylinder Wall

Piston

Drive Mechanism

\( \rho_i \) (avg. piston speed)

\( v \) (avg. discharge velocity)

Expelled Volume at \( \rho_0 \)

\( \Delta p \)
Assuming incompressible flow and cancelling density on both sides of the equation:

\[
\left( \frac{\text{flow speed thru opening}}{\text{valve area}} \right) = \left( \frac{\text{piston area} \times \text{mean piston speed}}{\text{valve area}} \right) \tag{2.2}
\]
or

\[
v = \frac{(A_p \times u)}{A_v} \tag{2.3a}
\]

where \( v \) is gas velocity, \( A_p \) is piston face area, \( A_v \) is the average valve opening area, or aperature, and \( u \) is the average piston speed.

To account for the compressibility of the gases, a mean flow coefficient is used, \( C_i \), which is representative of valve design and operation and accounts for the resistance to flow. Since \( C_i \) is always less than unity, it indicates a much faster exit flow velocity for compressible fluids:

\[
v = \frac{(A_p \times u)}{(A_v \times C_i)} \tag{2.3b}
\]

Now, the ratio of piston face area to average valve opening \( (A_p/A_v) \) is expressed simply as \( A \), and the actual flow rate compared to the maximum, sonic flow rate, \( a_s \), is the Mach index, \( Z \):

\[
Z = \frac{(u \times A)}{(C_i \times a_s)} \tag{2.4}
\]

The most important of these parameters, the one most affected by valve design, is the mean flow coefficient, \( C_i \). This value ranges from about 0.3 for cam-operated poppet valves to 0.8 for sleeve valves. The maximum for \( C_i \) would be 1.0, so sleeve valves, if they can be used, hold a lot of promise for reducing flow losses.
As for mean piston speed and sonic velocity, these can be calculated as follows:

\[ u = (2 \times s) \times \left( \frac{\text{RPM}}{60} \right) \times B \]  

where \( B \) is the number of cycles per revolution and \( s \) is the stroke (in inches).

\[ a_s = \sqrt{Y \times g_c \times R \times T} \]  

where \( T \) is the gas temperature, \( R \) is the gas constant, and \( g_c \) is a conversion constant. (Note that \( B \), the number of cycles per revolution, is determined by the physical design of the piston arrangement. Four-stroke engines have two revolutions per cycle, with one stroke up and one stroke down per revolution, and require two revolutions to complete the intake-compression-expansion-exhaust process. The PACE design, depending on the gearing arrangement, can have any number of cycles per revolution. The first PACE design, with its trichoidal cam housing, had three cycles per revolution).

Taylor [12] presents ample evidence of the dependency of pressure losses on the Mach index. Rosa [4], however, has compiled Taylor's data into a simple equation which can be used to determine the pressure drop across inlet valves for IC engine cylinders.

\[ p = p_r \times (1 - 1.25 \times z^2) \]  

where \( r \) is a subscript for \( r \) reservoir pressure and \( p \) is the back pressure.
Although this relationship holds for IC induction processes, Rosa suggests using the same equation for exit losses, acknowledging that Eq 2.7 is likely to overpredict losses in this case. The point is, there is no simple relationship to determine pressure drop across valve openings. Clearly, there is a dependency upon the Mach index, and a fit to a square relation is not unreasonable, especially since pressure drop across orifices is a function of the square of the velocity. How the mean flow coefficient, $C_i$, may change with speed, and pressure ratio is also not well established but may be assumed constant for a particular engine design. Pressure drop across valve openings is discussed in the model development in Chapter 3, Section 3.3.2.

In summary, good valve design is critical in reducing pressure losses. Regardless of whether the valve is cam- or pressure-operated, minimizing flow resistance and maximizing port area and duration of valve opening helps to ensure minimum pressure loss. In IC engines, inlet and exit valve openings may overlap and may not necessarily be timed at the beginning or end of piston strokes. Valve overlap, timing, and aperture is a design problem in itself and well beyond the scope of this thesis. Usually, these design aspects are optimized to take advantage of blowdown or working fluid inertia to aid in gas discharge, induction, or mixing.
2.4 Volumetric Efficiency, Expander Admission Coefficient, and Mass Recirculation

Volumetric efficiency in piston compressors and four-stroke engines is defined as the ratio of actual mass inducted during the intake stroke to the ideal mass which would fill the swept volume of the cylinder at ambient conditions:

\[ e_v = \frac{M_{\text{actual}}}{M_{\text{ideal}}} \]  \hspace{1cm} [2.8]

\[ M_{\text{ideal}} = \rho_i V_C \]  \hspace{1cm} [2.9]

\[ M_{\text{actual}} = \rho_a (V_C + V_{cv} - V_e) \]  \hspace{1cm} [2.10]

where \( \rho \) is density, \( V_C \) is the swept volume, \( V_{cv} \) is the clearance volume, \( V_e \) is the expanded volume of the residual gases, and subscripts \( i \) and \( a \) are for ideal and actual, respectively.

If the densities of the ideal mass and actual mass are the same, the volumetric efficiency becomes a volumetric ratio. In the absence of heat transfer and the pressure losses induced by piston speed effects, this is truly the case and EQ 2.8 becomes:

\[ e_v = \frac{\rho_i V_C}{\rho_a (V_C + V_{cv} - V_e)} \]  \hspace{1cm} [2.11]

The subtracted value on the right hand side of EQ 2.11 accounts for the displaced volume in the inducting cylinder which is occupied by the clearance volume residual gases at the end of the discharge stroke. Without this reexpansion of residual gases, volumetric efficiency would be very high. Many sources [14, 15] use a form of EQ 2.11 for
calculation of volumetric efficiency, ignoring heat transfer and pressure drop (density reduction) effects. For low speeds, with good valve "breathing", EQ 2.11 is a good approximation.

Taylor [12], on the other hand, derives volumetric efficiency based on thermodynamic properites and conditions of the residual and inlet gases. The equation for calculating volumetric efficiency for the PACE compressor, derived in Appendix A, is based on Taylor's energy balance analysis.

Volumetric efficiency is an important factor affecting engine power in four-stroke IC engines. The reason is straightforward: power is directly proportional to gas throughput (air handling capacity) per cycle. If all other influences were held constant, higher volumetric efficiency would produce higher power output. If one could attain the same mass flow rate and enthalpy exit conditions from the PACE compressor at a lower RPM, the friction losses would be proportionately less and net specific work would be larger.

Alternately, since friction is relatively independent of mass flow, by increasing volumetric efficiency at a given RPM, net work is higher and friction remains constant. The effect is to increase thermal efficiency. Therefore, volumetric efficiency can be a significant factor in engine thermal efficiency.

Volumetric efficiency is affected strongly by valve timing, cylinder clearance volume, gas temperature and pressure, heat transfer during induction, and, most importantly, piston speed. Taylor's data shows that at Mach index values of $Z$ greater than 0.6, the volumetric efficiency drops off dramatically. His recommendation to designers is
to keep piston speeds low enough, and valve opening areas high enough, to minimize the Mach index value.

Recirculation of the residual gases trapped in the clearance volume of the compressor cylinder has a pronounced effect on volumetric efficiency; the larger the clearance volume the more dominant the effect. Since residual gases in a compressor cylinder are at high pressure at the end of the discharge stroke, these gases expand beyond the clearance volume in the downward, induction stroke. The greater the volume occupied by the recirculated residual gases, the less volume available for a new charge to occupy—lowering volumetric efficiency (see EQ 2.11).

For two-stroke engines, volumetric efficiency is not a meaningful performance indicator because the cylinder induction and discharge processes overlap and cannot be distinguished. In two-stroke engines there is considerable mixing of residual gases with the incoming charge. A scavenging coefficient is a more appropriate index used for two-stroke engines, indicating the effectiveness of the engine in expelling residual gases.

Similarly, expanders cannot be characterized adequately by volumetric efficiency because the intake part of the induction stroke is only a portion of the entire expansion stroke, expanding to a partial "intake" volume, \( V_I \) (see Fig. 2.1). The rest of the downward stroke of the expander, after the intake valve closes, is the actual expansion portion. Therefore, we define an "admission coefficient", \( n_a \), for the expander (in Appendix A) which can be used to determine the charge admission effectiveness of the expander.
In the PACE expander, residual gases become a problem because they must be recompressed to equal intake pressure if pressure losses are to be reduced. Alternately, the residual expander gases can be left at discharge pressure (nearly atmospheric) but the relative pressure between intake and residual is large (on the order of the pressure ratio for the compressor). This issue is not resolved in the literature, but it appears that even if residual gases were not recompressed, the pressure drop at inlet may not be significant since the piston is at zero velocity at TDC before it begins the intake. The Mach effect would, therefore, be insignificant. In either case, residual gases in the expander lower the value of the expander admission coefficient, but not nearly as dramatically as the expansion of the compressor residual gases lowers volumetric efficiency.

2.5 Heat transfer

Much has been written in the literature about heat transfer. Both Obert [17] and Taylor [12] provide comprehensive general summaries on the subject. Taylor, especially, has compiled a breadth of results from heat transfer studies by other researchers as reported in the technical literature on IC engines.

Heat transfer in IC cylinders is inherently complex. It can be characterized by its cyclic nature, its varying geometry, pressures, and temperatures, and its discontinuous gas exchange profile, not to mention the heat transfer property differences among its non-uniform contact surfaces.
In trying to find a concise analytic form for heat transfer from an engine cylinder, several authors [2, 13, and 18] have treated it as a cyclic phenomenon with the cylinder walls storing and then regenerating heat. The idea is that the working fluid, which is relatively cool, absorbs heat upon induction, becomes very hot during combustion, and then discharges heat to the cylinder walls through the end of the exhaust stroke. There is a net heat transfer out of the cylinder because the average temperature of the walls is much higher than the temperature of the coolant on the other side of the cylinder walls.

The main problem with adapting this concept and its various forms to the PACE model is the fact that there are too many coefficients in the cyclic heat transfer equations to be manageable for a parametric model. Each coefficient requires empirical data for the equations to be useful. The thermal diffusivity value \((\alpha = \frac{k}{\rho c})\) only comes into consideration when a cyclic analysis is used; \(k\), \(\rho\), and \(c\) are the conductivity, density, and heat capacity, respectively, of the material. In principle, the thermal diffusivity is but a conductivity value, modified by a material's density and thermal storage capacity. The higher the value used for either of these last two properties, the smaller the thermal diffusivity and the less the heat stored and regenerated. Decher [13] emphasizes that the heat storage, and therefore the cyclic heat losses, can be reduced by minimizing the quantity \(\sqrt{\frac{k}{\alpha c}}\).

Also important is the point made by Colgate [18] that the real heat transfer problem may not be the net loss through the cylinder walls but the irreversible storage and reabsorption of heat as the gas is
alternately compressed then expanded. The implication is that no matter how well insulated the cylinder walls, heat transfer losses will be significant due to the out-of-phase heat exchange. Accounting for such a time-varying irreversibility would require empirical data and is beyond the scope of the steady-state model developed in this thesis.

Another approach to solving the heat transfer problem is to treat the heat transfer as a total quantity or rate. This simplifies the analysis, and fewer parameters need to be estimated. Still, empirical data is needed for validation of equations applicable to IC engines, if these equations are to be adapted for PACE engine analysis.

Obert [17] develops the heat transfer relationships for forced flow in a cylinder from first principles. Taylor's development [12] is similar to Obert and both arrive at a basic relationship:

\[ \frac{h_b}{k} = C \cdot Re^n \cdot Pr^m \]  \[2.12\]

where \( b \) is the bore; \( h \) and \( k \) are the gas convective and thermal conductivity heat transfer coefficients, respectively; \( Re \) is the Reynolds number; \( Pr \) is the Prandtl number; \( C \) is a proportionality constant, and \( (h_b/k) \) may be recognized as the Nusselt number.

In all cases, the \( m \) and \( n \) exponents are characteristic of the flow regime and the physical characteristics of the cylinder arrangement. Empirical values for \( n \) range between 0.5 and 0.8. Since the Prandtl number is very nearly constant for gases over a broad range of temperature EQ 2.12 reduces to:

\[ \frac{h_b}{k} = K \cdot Re^n \]  \[2.13\]

where \( K = C \cdot Pr^m \)
Next, Taylor describes three simultaneous equations to define the heat flow: from working fluid to the cylinder wall; through the wall; and from the wall to the coolant. Then, Taylor defines an overall heat transfer coefficient:

\[ h_e = (\dot{Q}/A_p) \times (T_g - T_c) \]  \[ 2.14 \]

where \( T_g \) is the mean effective gas temperature over a cycle, \( T_c \) is the average coolant temperature, and \( \dot{Q} \) is the heat loss rate to the coolant. \( A_p \) is a reference area, the piston face. Note that \( h_e \) is not the same as a convective film coefficient, but an empirical composite heat transfer coefficient. Harkening back to EQ 2.12, Taylor suggests that \( h_e \) can be expressed in a similar relation:

\[ h_e b/k = f(Re) \]  \[ 2.15 \]

\[ Re = (G b)/(\mu g_c) \]  \[ 2.16 \]

where \( G \) is the mass flow rate per piston area and \( \mu \) is the dynamic viscosity. Since EQ 2.15 is a steady state relation, it does not account for heat storage effects, and it masks all transient conditions during a cycle by lumping the heat transfer characteristics into average values.

Empirical data from hundreds of heat transfer studies for IC engines reveal that EQ 2.15 can be described as:

\[ h_e b/k = 10.4 \times Re^{0.75} \]  \[ 2.17 \]
The implication of this result is that heat transfer can be calculated using Eq. 2.17 as long as the coolant and mean effective temperatures are known. This simplifies the heat transfer analysis tremendously. Substituting Eq. 2.17 back into Eq. 2.14, an overall heat transfer equation is derived.

It is noteworthy that this relation holds for two- and four-stroke engines, over a broad range of RPM and varying bore/stroke ratios. It is also important to note that the thickness and conductivity of the cylinder wall material (typically steel or aluminum alloys) has little effect on this overall relationship. The driving, overriding factor in heat transfer in reciprocating piston cylinders is the Reynolds number.

2.6 Friction

Mechanical friction in piston engines is expressed as friction mean effective pressure (fmep) over an entire cycle. By dividing the fmep by the number of strokes per cycle, then multiplying by the volume displacement per cycle, one can determine the displacement work per cycle, or rate of friction work. Taylor [12] derives this as follows:

\[ \dot{W}_f = \frac{(\text{fmep} \times A_p \times u)}{S} \]  

[2.18]

where \( \dot{W}_f \) is the power, or load, absorbed by friction, \( S \) is the number of strokes per cycle, and \( A_p \) and \( u \) have been previously defined.

Taylor presents evidence indicating fmep to show very nearly a direct linear relation to average piston speed, such that:

\[ \text{fmep} = f \times u \]  

[2.19]
The value of $f$, the friction coefficient, is peculiar to engine type, and is higher for two-stroke engines than for four-stroke, and higher still for four-stroke Diesels than gasoline engines. Two-stroke engines have inlet and outlet ports at the end of the expansion and beginning of the compression strokes. Less of the stroke length is used for expansion or compression compared to four-stroke engines which are almost all expansion or compression for the entire stroke. Also, both the up and down strokes of a two-stroke engine operate under load, whereas only two of four strokes are loaded for four-stroke engines. In general, higher internal gas pressures induce greater ring resistance. Therefore, Diesels, with high compression ratios, tend to exhibit the greatest $f_{\text{me}}p$ values.

Mechanical friction includes friction of both the piston rings and the bearings and valve system, but piston rings typically are responsible for about three-quarters of the friction losses. According to Taylor [12], friction is proportional to bearing area. Therefore, the larger the piston circumference, the greater the $f_{\text{me}}p$.

Although quantitative relations for determining $f_{\text{me}}p$ as a function of piston circumference or mean cylinder pressure are not given by Taylor, Rosa [4] poses the following equation, curve fit from Taylor's data, to accommodate the pressure influence:

$$f_{\text{me}}p = 7 + \frac{u}{200} + \left(\frac{u \cdot \bar{p}}{17,600}\right)$$  \[2.20\]

where $\bar{p}$ is mean pressure in psig, $u$ is in ft/minute, and $f_{\text{me}}p$ is in psia. The value of $\bar{p}$ is determined from a "volume averaged" pressure, which assumes equal cylinder volumes are swept in equal amounts of time.
Experimentally, the fmep value is determined by disconnecting the engine load and closing off cylinder valves, then compressing and expanding the cylinder charge without firing it and without gas exchange. Because this approach would be equally applicable to IC engines and to the PACE, Rosa proposes EQ 2.20 as suitable for calculations in a reciprocating Brayton cycle engine analysis.

A note of caution is appropriate here. Rosa’s EQ 2.20 must be taken with a grain of salt. In IC engines, fmep accounts for 5% - 20% of the overall mep. But if one can assume, as Rosa did, that fmep for a PACE-type engine would be the same as that of an IC engine with the same stroke at the same RPM, the percent fmep predicted by EQ 2.20 would be unacceptably high. This caution is even more important when one realizes that power densities of IC engines are likely to be much higher than those for the PACE for several reasons, including the fact that working fluid densities in the PACE combustor will be much lower and the pressure-temperature profiles of the two types of engines are quite distinct.

2.7 Compressor and Expander Component Efficiencies

In any discussion of overall Brayton cycle engine efficiency, the question of individual component efficiencies, for both compressor and expander, always comes up. Typically, a turbine or an axial compressor, for example, is given an "adiabatic" efficiency provided by the
manufacturer. Adiabatic efficiency is defined as follows for compressor and expander components, respectively:

\[ e_c = \frac{(h_2 - h_1)}{(h_{2s} - h_1)}; \text{ (ideal work/actual work)} \]  \[2.21\]

\[ e_E = \frac{(h_3 - h_{4s})}{(h_3 - h_4)}; \text{ (actual work/ideal work)} \]  \[2.22\]

In Eqs 2.21 and 2.22, the subscript "s" indicates the actual end points for the compressor and expander irreversible processes (see Fig. 2.3), which is an increase in entropy relative to the ideal isentropic process. Note that the values are for specific enthalpy, in BTUs per lbm.

The discussion which follows focuses on compressors, but the arguments and the development of equations apply equally well to piston expanders. The first question which arises is how to accommodate non-adiabatic compression processes. Lee and Smith [2] note that whenever net heat transfer is introduced, Eq 2.21 is modified to be:

\[ e_c = \frac{(h_2 - h_1)}{[(h_{2s} - h_1) + \dot{Q}/\dot{m}]} \]  \[2.23\]

The significant point to keep in mind is that the value \( h_{2s} \) in Fig. 2.3 is for an adiabatic process where the irreversibilities are not due to heat transfer, but to pressure losses, fluid friction losses, and inefficient momentum transfer. Furthermore, First Law analysis shows that the increase in enthalpy of the exit stream of the compressor, in a steady state, steady flow process, is a result of the total work input minus the heat loss:

\[ \dot{m} * (h_{2s} - h_1) = \dot{W} - \dot{Q} \]  \[2.24\]
Fig. 2.3 -- h-s Diagram for the Brayton Cycle
Here, the sign convention is positive for work into and negative for heat out of a system. Clearly, Eq 2.21 cannot be relied upon for calculating actual work per cycle in the compressor without also knowing the heat transfer, unless \( \dot{Q} \) is assumed to be negligible.

Many authors [13, 21] attempt to determine an overall compressor efficiency using the "polytropic" exponent method to account for all the irreversibilities. The polytropic exponent is defined as:

\[
n = \frac{(Y-1)/\varepsilon Y}{(E_Y-1)/(E_Y)}
\]  \[\text{[2.25]}\]

where \( \varepsilon \) is the polytropic factor.

Then, the compressor component efficiency follows:

\[
e_C = \frac{(R_C \sigma - 1)/R_C^n - 1}{(R_C \sigma - 1)/(R_C^n - 1)}
\]  \[\text{[2.26]}\]

\[
h_{2s} - h_1 = c_p \cdot T_1 \cdot (R_C^n - 1)
\]  \[\text{[2.27]}\]

where \( \sigma = (Y-1)/Y \) and \( R_C \) is the pressure ratio.

Since constant-temperature lines parallel constant enthalpy lines on a h-s diagram for a perfect gas, any irreversible process ends up at a higher temperature than the reversible one. So, an adiabatic efficiency does not account for heat transfer because actual working fluid temperature is lower than adiabatic temperature. In other words, the end point \( h_{2s} \) on the h-s diagram represents the actual thermodynamic state of the working fluid at the end of an actual compression process only if there is no heat transfer.

If one wanted to represent actual compressor processes on Fig. 2.3, then the end point \( h'_{2s} \) would indicate the thermodynamic state...
of the working fluid without heat transfer, and the difference (h_{2s}' - h_{2s}) accounts for the heat transfer during compression.

Scheel [14] and Oates [21] contend that the polytropic efficiency is best applied to multi-stage systems, such as axial compressors, where the compression process is truly polytropic.

Scheel provides a comprehensive method for determining compressor efficiency, accounting primarily for pressure drops at the valves and ignoring friction and heat transfer losses. Scheel makes the point that in piston compressors the actual compression is very nearly adiabatic, but the critical irreversibilities arise from the valve losses experienced during admission and discharge. This may not be the case for expanders, where heat transfer may be quite significant due to higher temperatures compared to those in compressors.

In an attempt to accommodate irreversibilities due to speed effects, Tsongas and Jellesed [20] modeled adiabatic compressor efficiency as a quadratic relation.

\[ e_c = e_c' \left[ 1 - a\left(\frac{u}{u_{\text{max}}}ight) - b\left(\frac{u}{u_{\text{max}}}ight)^2 \right] \]  

where \( e_c' \) is a reference efficiency, \( a \) and \( b \) are empirical coefficients, \( u \) is average piston speed and \( u_{\text{max}} \) is the reference maximum piston speed of 3000 ft/min.

This approach does not rely on a polytropic exponent. The square term with the coefficient \( b \) actually approximates pressure loss effects which are proportional to the square of the mean piston speed, while the linear term, with the coefficient \( a \), may well account for mechanical friction. Heat transfer, as has been reviewed in a previous section, is
inherently much more complex. In any case, good curve fits to empirical data to derive Tsongas' coefficients, a and b, would be a very direct way to develop a foundation for a parametric analysis model.

2.8 Summary

The literature provides background and discussion about how the identified irreversibilities in IC engines are treated. Except for the two engine designs discussed which are similar to the PACE, the literature does not describe a comprehensive framework for treating the unique characteristics of the PACE design. However, data from IC engines can be extrapolated, where applicable, to develop an analytic model for the PACE. More importantly, the PACE model developed in the next chapter is a composite of equations adapted from the literature and assumptions must be made to use them. This is one limitation of all models, but one which must be reckoned with.

Clearly, the pressure and temperature profiles of a four- or two-stroke IC engine are not even comparable to the PACE design with its separate compression, expansion, and heat addition components. In the IC engine these processes are all combined into one cylinder. Lack of empirical data on the temperature and pressure profile effects on valve losses, friction, and heat transfer does not hamper developing the analytic framework for this model. But it does underscore the need to have good empirical input data for the model in order to obtain realistic results.
To summarize, the important irreversibilities associated with the PACE compressor and expander components are pressure losses, heat transfer, and friction. Both the compressor and expander do flow work to move the working fluid through the cylinders, especially at the inlet and exit ports. All irreversibilities have been shown to be functions of at least two key parameters: piston speed and pressure ratio. Friction is primarily speed dependent, heat transfer depends on working fluid density and mass flow rate (related to pressure ratio and piston speed), and pressure losses are proportional to square of the average piston speed. Mass losses, although not discussed in this chapter, also account for reductions in power and efficiency. But this problem is dealt with analytically in Chapter 3.
CHAPTER 3

ANALYTICAL METHODOLOGY

All the work referenced in Chapter 2 is developed in this chapter into equations which become the basis for the software model. The discussion focuses first on a descriptive review of the basic PACE engine design and the thermodynamic processes of the compressor, combustor, and expander. Each of the identified irreversibilities is developed in detail and equations are presented which are used in the software algorithms that define engine performance. The chapter ends by discussing the rationale, usefulness, and limitations of a parametric analysis model.

The analysis of the PACE engine performance is divided into three basic processes: compression, heat addition, and expansion. In this project, the major emphasis is on the PACE compression and expansion, and the heat addition will be dealt with only in an elementary fashion. Compression is divided into admission, compression, discharge, and reexpansion of residual gases. Similarly, the expander processes are intake, expansion, exhaust, and recompression of residual gases. In principle, the expander's operation is just the reverse of the compressor, except it sees much higher temperatures at lower gas densities.
Although the compressor and expander components are treated separately, both have a similar analytic foundation. Both are modeled as two-part components, with an adiabatic part and a heat transfer part. The approach taken in this chapter is to analyze the adiabatic part first, including the pressure loss irreversibilities during induction and discharge of the compressor and during intake and exhaust of the expander. The actual expansion and compression processes are modeled as adiabatic and reversible in these two components. Then, the heat loss irreversibility is included and friction losses are added. Mass loss is calculated using a modified polytropic exponent, as described in Section 3.8, then an average total mass is used to determine mass flow rate through the compressor and expander to calculate net specific work and power.

3.1 Assumptions and Initial Considerations

All computer models, regardless of their degree of complexity, are essentially mathematical abstractions, and the underlying equations only approximate real conditions. No model can possibly account for every detail and characteristic of the system it represents. Some simplifications are necessary to make the model manageable, both mathematically and in terms of the complexity of the computer analysis needed for calculations.

However, important operating and design characteristics can be identified and the key parameters which influence these characteristics can be specified. A model becomes a kind of "black box": in goes a set
of input data and output the results which describe the engine's performance characteristics. Inside the black box is a set of algorithms which define the functional relationships and influences among all the input data.

Although this model has powerful analysis capability and the flexibility to deal with an enormous array of design and operating characteristics, its predictive ability and its results are only as good as the assumptions used to make the analysis manageable. The model's key assumptions are specified here. Later on, as other assumptions are encountered in the course of the chapter, these assumptions are discussed more fully and their impact on the accuracy of the model's results is considered. Other assumptions are discussed in the context of where they apply and how they influence the analytic basis for the model. As a foundation for the PACE engine model, the following assumptions are made:

1. Constant (average) specific heats are used for all processes. A value of constant pressure specific heat \( c_p \) and other properties for air will be used up to the point of combustion, then new values for the combustion gases can replace these values in the calculations. (See Obert [17], p.732 for data on specific heats of air).

2. The perfect gas law applies to the working fluids where \( pV = MRT \). Compressibility factors and pressure tables are not used. Key thermodynamic equations are derived based on this perfect gas relation.
3. Compressor work is analyzed as a two-part process. It is modeled as if it had an adiabatic component and a heat transfer component. The expander work is treated in the same way.

4. Heat transfer accounts for energy lost from the working fluid in the cylinders during compression or expansion. Heat loss is treated as a total quantity for an entire cycle for both compressor and expander. This irreversibility is calculated after the adiabatic work of compression or expansion has been calculated.

5. The heat generated by friction work is presumed lost without being reabsorbed into the working fluid, transferred directly to the cooling system. Friction is calculated as a mean effective pressure in compression or expansion, and treated as a net work loss per cycle, or load, for both the compressor and the expander.

6. All valves open and close instantaneously. The model assumes an average port area \( (A_i \text{ or } A_e) \) exposed for the inlet and exit of gases. Valves can be single or multiple, delta-p or cam operated. If multiple valves are used, their cumulative aperture area is treated as a single valve. If valves are not pressure-controlled, then it is assumed that control algorithms which mimic the operating constraints described in the model, such as pressure ratio, are responsible for valve operation.
7. All port expansion processes (pressure losses) are treated as isothermal, isenthalpic expansions—essentially a throttling process.

8. Mean inlet and exit flow coefficients ($C_i$ and $C_e$) are treated as constant for a particular design configuration. These are empirical values. Although they may vary with peak temperature, speed, or pressure ratio parameters, these influences have not been established in the literature and are not likely to significantly affect the pressure drops calculated using this coefficient, at least not as strongly as the piston speed affects pressure drop.

9. Empirical data, derived from studies of IC engines, will be used where appropriate information is lacking for corresponding aspects of the proposed PACE engine. In particular, data on friction, heat transfer, and pressure losses in IC engines will be assumed applicable to the PACE.

10. This engine model allows for either a variable volume expander (VVE) or variable speed drive (VSD) design option, but not both.

11. Flow regimes with working fluid velocity greater than Mach 1 are not allowed. The engine is constrained to operate at piston speeds below 3000 ft/min, which is the maximum found in the literature. The average piston speed does not exceed the sonic speed or 3000 ft/min, whichever is less. The engine is not expected to operate outside these reasonable constraints.
12. All analysis is for steady-state conditions; the model does not accommodate transient analysis.

3.2 Diagram and Description of the PACE Engine Model

We begin laying the groundwork for the algorithms used in the software model by describing the basic PACE engine as shown in Fig. 3.1. The diagram has three components: a compressor, a combustor (or heater), and an expander. The PACE engine, in principle, operates very much like an open Brayton cycle. The working fluid is compressed, heat is added at constant pressure, and then the working fluid is expanded to ambient pressure. Some of the work of the expander is used to drive the compressor. The PACE engine is similar to the gas turbine except the compressor and expander are reciprocating, constant displacement devices rather than aerodynamic, rotating machines. Table 3.1, below, identifies the thermodynamic state points. These numbers are also the subscripts for temperature and pressure.

<table>
<thead>
<tr>
<th>State Point</th>
<th>Thermodynamic Process</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>ambient air conditions</td>
</tr>
<tr>
<td>0 --&gt; 1</td>
<td>pressure drop at compressor inlet</td>
</tr>
<tr>
<td>1 --&gt; 2</td>
<td>compressor admission</td>
</tr>
<tr>
<td>2 --&gt; 3</td>
<td>compression</td>
</tr>
<tr>
<td>3 --&gt; 4</td>
<td>compressor discharge</td>
</tr>
<tr>
<td>4 --&gt; 5</td>
<td>overall heat loss in compressor</td>
</tr>
<tr>
<td>5 --&gt; 6</td>
<td>heat addition in combustor (heater)</td>
</tr>
<tr>
<td>6 --&gt; 7</td>
<td>expander intake</td>
</tr>
<tr>
<td>7 --&gt; 8</td>
<td>expansion</td>
</tr>
<tr>
<td>8 --&gt; 9</td>
<td>expander exhaust</td>
</tr>
<tr>
<td>9 --&gt; 10</td>
<td>overall heat loss in expander</td>
</tr>
<tr>
<td>10</td>
<td>exhaust gas conditions</td>
</tr>
</tbody>
</table>
Fig. 3.1 -- PACE Engine Model
For reasons already alluded to in the heat transfer discussion in Chapter 2, both the compressor and expander are modeled as two-component devices, having separate adiabatic and heat loss components. Fig. 3.2 is a diagram of the compressor. Because heat transfer can only be calculated, practically, as a total quantity, given certain operating characteristics, the heat transfer is separated and analyzed after the compression is completed. Likewise, the expander is treated in a similar way as shown in Fig. 3.3. This simplification will be addressed in greater detail in Section 3.6, dealing with heat transfer.

For purposes of this model the combustor is treated simply as a heat addition component. The model makes no distinction between an indirect-fired heat exchanger and a combustor. As will be explained in Section 3.4, the additional mass contribution of the fuel is a relatively insignificant proportion and is therefore neglected. Since combustion processes are not modeled in this thesis, a combustor is synonymous with a heater. So the heater or combustor will be referred to simply as a "combustor" throughout this thesis.

Before getting any deeper into the analysis, there are a few other noteworthy points to mention about Fig. 3.1. Note that all the sources of irreversibilities are identified: heat transfer (HT), pressure losses (PR), friction (FR), and mass loss and recirculation (MA). Also note that the important working fluid properties are segregated into two sets of average values: those for the working fluid prior to heat addition, and those afterward (designated by the prime notation). These properties are average values of specific heats \( c_v \) and \( c_p \) (both constant volume and constant pressure), dynamic viscosity \( \mu \), gas
Fig. 3.2 -- PACE Compressor Model Diagram

Fig. 3.3 -- PACE Expander Model Diagram
conductivity \((k)\), modified polytropic expansion and compression exponents \((n)\), and gas constants \((R)\). The significance and application of each of these properties will be explained as they are encountered in the discussion which follows.

In summary, the approach taken is to first evaluate the compressor, as well as the expander, processes as if they were adiabatic, accounting only for pressure losses. Once the thermodynamic conditions of the working fluid are known, these values are used to estimate the heat transfer rates from the compressor and expander. Mass loss is then calculated. Lastly, friction is included to complete the analysis of component performance. Friction is treated as an independent load against which the pistons work. A review and analysis of \(p-V\) diagrams for the PACE compressor and expander components graphically illustrates the engine's thermodynamic processes and irreversibilities. We start with the compressor.

### 3.3 The PACE Compressor--Adiabatic Compression with Pressure Losses Only

First we treat the compression process as if it were adiabatic, without friction, heat transfer, or mass loss. Since both heat transfer and mass leakage from a compressor cylinder is relatively small, this is a good first approximation for analyzing compressor work over a cycle. Heat transfer and mass loss are addressed later in this discussion as the model becomes more refined.

Fig. 3.4 is the \(p-V\) diagram for the compressor processes. Three separate processes are shown for comparative purposes. A light line
Fig. 3.4 -- PACE Compressor p-V Diagram
a'-b'-c'-d'-a' represents the idealized, isentropic compression process without pressure losses or heat transfer. The process takes place between the pressure limits \( p_3 \) and \( p_0 \), and between the clearance volume, \( V_{cv} \), and \( V_2 \).

In contrast, the compressor process being modeled here as a first approximation includes pressure losses but excludes heat transfer, friction, and mass loss. This is indicated by the dark solid line a-b-c-d-e-a. Lastly, the dotted line represents an actual compressor cycle a-b'-c'-d'-e'-a. The only difference between the dotted line and the dark solid line is heat transfer. The area differences between the ideal and the actual cycles indicate lost or excess work attributable to loss of available energy due to heat transfer and pressure losses.

For the compressor process under consideration, \( p_4 \) is the discharge pressure, \( p_3/p_0 \) is the design pressure ratio, \( R_c \), and \( p_0 \) is ambient pressure. \( V_C \) is the swept volume, equal to \((V_2 - V_{cv})\). Note that the operating discharge pressure is actually \( p_4 \), as modeled, but \( p_3 \) is the compressor design pressure. This is because the software model treats \( p_3/p_0 \) as a nominal pressure ratio and uses \( p_3 \) to simulate the threshold control pressure for the opening of the discharge valve.

3.3.1 PACE Compressor Expansion of the Residual Gases

In Fig. 3.4, we can trace the piston travel through one cycle, beginning at point a, which is top dead center (TDC) at the end of discharge. At point a, the residual gas in the cylinder is at the
discharge temperature and pressure \( (T_4 \text{ and } P_4) \) and occupies the clearance volume, \( V_{cv} \).

In all cylinders, there is some clearance volume—on the order of 5-20% of the cylinder swept volume—where there is always some residual gas left in the cylinder at the end of discharge. In other IC engines, the clearance volume provides a space for the actual charge explosion. But more importantly, the clearance volume is dictated by the compression ratio the fuel can tolerate without experiencing knock, or autoignition. In the PACE, conceivably, there need be no clearance volume since there is no air-fuel mixture in the compressor cylinder and no potential for knock. Compression ratios could be increased dramatically beyond conventional bounds, limited only by the pressure strength of the cylinder and piston. As will be seen from the results reported in Chapter 5, minimizing the clearance volume enhances the engine performance in many instances. PACE clearance volume can be very small, especially if there is no need for clearance space for valve components.

Getting back to the compressor, the residual gas in the clearance volume expands as the piston begins its downward stroke. In this model, this expansion is treated as an isentropic process from point a to b. (If heat transfer were to be included, the actual profile of the process would be a-b" which is less steep and could be modeled as a polytropic, rather than isentropic, expansion. The residual gas is at a relatively higher temperature than the average cylinder inner surfaces, so there would be a net heat loss and therefore a loss of expansion work).
The equations describing the adiabatic, reversible expansion, relating both pressure and volume are:

\[ pV^Y = \text{constant} \quad [3.1] \]

\[ \frac{V_{cv}}{V_1} = \left(\frac{p_1}{p_4}\right)^{1/Y} \quad [3.2] \]

where \( Y \) is the ratio of specific heats. The pressure at \( p_1 \) is something less than ambient. This is due primarily to pressure losses through the inlet manifold, but also to the differential threshold pressure which may be required to open the inlet valve if the valve is pressure operated. Valve design and operation are obviously an important design factor, as has been discussed in Section 2.4. This model assumes an average port area for the inlet valve, and the inlet valves are assumed to open instantaneously at point b.

Without a clearance volume, the PACE compressor could compress to an infinitesimally small volume, with corresponding very high pressure ratios (or compression ratios). Of course, if there is a clearance volume, the pressure ratio is limited by the following relation:

\[ R_{C(\text{max})} = \left(\frac{p_3}{p_0}\right) < \left[\frac{V_{cv} + V_C}{V_{cv}}\right]^Y \quad [3.2a] \]

And if the proportion of clearance volume to swept volume can be expressed as a ratio \( x = \frac{V_{cv}}{V_C} \), then Eq 3.2a becomes:

\[ R_{C(\text{max})} < \left[\frac{(x + 1)/x}{x}\right]^Y \quad [3.2b] \]
If \( x \) were to go to zero, then the pressure ratio could, theoretically, go to infinity, since the mass could be squeezed to even smaller and smaller volumes.

### 3.3.2 PACE Compressor Admission Process

At point \( b \) the admission process begins, and air is drawn into the cylinder by the relative vacuum created as the piston increases the cylinder volume. When the admission valve opens, the new charge rushes in, mixing with the residual gas, and begins to fill the cylinder. The rate at which the new charge enters the cylinder is critically dependent upon the port opening area and piston speed. Note that the new air charge entering the piston is not at ambient temperature — it tends to absorb heat in the entry manifold. However, it is treated in this case as if it were since heat transfer is dealt with as a separate problem. The faster the piston speed, the greater the pressure differential across the inlet port. The pressure drop is really dependent on the square of the piston speed. The exact relationship between pressure drop and piston speed is very complex but it is modeled here in the same manner as Rosa [4] treated it, as was discussed in Section 2.4.

\[
\frac{p_0 - p_1}{p_0} = 1.25 \times Z^2
\]  

[3.3]

where \( Z \) is defined in EQ 2.4. In this model, the pressure drop is calculated as an average value from \( b \) to \( c \). The pressure at \( c \), at the end of admission, is assumed to be the same as the average pressure during the entire admission process from \( b \) to \( c \). The exact end-point
pressure at the end of the admission stroke is indeterminate but clearly must be less than admission but higher than the maximum pressure drop. $p_2$ defines the state of the air at the beginning of the compression stroke. In this adiabatic model, we assume the air enters the cylinder and expands isenthalpically, and therefore the temperature at $c$ is equal to the temperature at $b$, $T_2 = T_1$ (see Table 3.1 for state point subscripts). We also assume that the inlet valve closes instantaneously at bottom dead center (BDC).

Looking at the geometry of the admission process, it becomes clear that the volume to which the residual gases expand, $V_1$, limits the volumetric efficiency since $(V_2 - V_1)$ becomes the maximum fill space for the incoming charge. Volumetric efficiency determines how much mass the compressor will process per cycle. Both pressure drop during admission and the net effect of the manifold heat added in actual cycles contribute to reducing volumetric efficiency. Volumetric efficiency is given as

$$ e_v = (y((Y - 1)/Y) + (y \ast r - 1)/[Y(r - 1)]) \ast [(V_2 - V_1)/V_C] $$

[3.4]

where $r$ is $(V_2/V_1)$ and $y$ is $p_2/p_1$.

EQ 3.4 is derived in Appendix A and accounts for a mass and energy balance which depends on the thermodynamic states of both the residual gases and the inlet gases, and also accounts for pressure drops due to speed effects. Again, at this point in developing the model, adiabatic processes are assumed because heat transfer is dealt with separately.
3.3.3 PACE Compressor Compression Process

At BDC, which is point c, the inlet valve closes and the piston begins its compression of the mixed charge. In this model, the compression stroke is treated as isentropic and the relationship of \( EQ \ 3.1 \) applies.

As a comparison, compression in actual cycles is not quite adiabatic. The gas heats up during the compression stroke (c-d") and there is a net transfer of heat out of the cylinder. The net effect of this non-adiabatic behavior is to cool the gas relative to an adiabatic compression temperature. This reduces the enthalpy of the gas at the end of compression. The end pressure is the same in both cases, but the specific volume differs.

3.3.4 PACE Compressor Discharge Process

At some point d, the exhaust valve opens and the gas begins to discharge. Point d is fixed by the pressure ratio, \( R_2 \), which is an independent operating parameter that can be adjusted by some engine control mechanism. The pressure differential between points d and a \( (p_3 - p_4) \), is the driving potential to discharge the compressed charge. The compressor discharge pressure, \( p_4 \), is a function of the piston speed and port characteristics embodied in the parameter, \( Z \). We use Rosa’s approach and treat the pressure drop across the exit port in the same way as the inlet port:

\[
\frac{(p_3 - p_4)}{p_3} = 1.25 \times z^2 \quad [3.5]
\]
and

\[ T_3 = T_4 \]  

[3.6]

which assumes isenthalpic conditions.

Excess work is required to drive the compressed charge out of the cylinder. The "hump" profile between d and e depends primarily on engine speed and port configuration. Again, the Mach index, \( Z \), is the critical factor which is used to calculate the degree of excess work required as indicated by the pressure drop. We assume that the pressure, \( p_4 \), at the end point (a) is \( p_3 \) minus the average pressure drop.

3.4 Heat Addition

After the compressed air is discharged from the compressor, heat is added continuously to the charge at approximately constant pressure. The heat addition component is represented by either a combustor or a heat exchanger heater as shown in Fig. 3.1. There is some pressure drop due to flow losses through the combustor. Pressure drop is a function of the square of the mass flow rate, and is dependent on combustor port geometry. To simplify the model, this drop is treated simply as a percentage of total pressure.

Once inside the combustor, an amount of fuel \( (m_f) \) with a lower heating value LHV (BTU/lbm), is supplied at a continuous rate, combining with the high pressure air from the compressor in a constant pressure combustion process. In our model, we assume a fixed combustion
efficiency ($e_H$) and do not try to model the combustion process itself. EQs 3.7a through 3.7d model the heat input, $Q_H$, from combustion:

$$\dot{Q}_H' = \dot{m}_f * \text{LHV} \quad [3.7a]$$

$$\dot{Q}_H = e_H \cdot \dot{Q}_H' = [(\dot{m}_f + \dot{m}_C) \cdot c_p \cdot (T_{max} - T_5)] \quad [3.7b]$$

where the prime denotes the ideal heat input and $T_{max} = T_6$. If $\dot{m}_f$ is known, then the maximum temperature, $T_{max}$, can be determined.

Now, to determine the quantity $\dot{m}_f$, we need to know both the air-fuel ratio ($A/F$ in lbm-air/lbm-fuel) and the equivalence ratio, $\Phi$.

$$\dot{m}_f = \frac{\dot{m}_C}{(A/F \cdot \Phi)} \quad [3.8a]$$

The A/F ratio is the quantity of air, in lbm, supplied per lbm of fuel. Stoichiometric air-fuel ratios range from about 7 to 20 for hydrocarbon fuels. If the A/F ratio is less than stoichiometric required for combustion, it is said to be a "rich" burn, and unburned hydrocarbons can be found in the exhaust. If the A/F ratio is just the opposite, then the burn is considered "lean". Equivalence ratio is the ratio of actual air supplied to stoichiometric air. Typically, values for equivalence ratio range between 1.5 and 2 because some excess air is required to ensure complete combustion or limit the maximum temperature. Excess air tends to mitigate hydrocarbon pollutants but also diminishes combustion efficiency and, therefore, must be carefully controlled.

Realistically, actual A/F ratios then range from 10 to 30, depending, of
course, on the fuel. If we assume a typical A/F ratio is about 20 and \( \Phi = 1.5 \), then EQ 3.8a becomes:

\[
\dot{m}_f = \dot{m}_c / (1.5 \times 20) \tag{3.8b}
\]

and EQ 3.7b becomes

\[
\dot{Q}_H = [1.03 \times \dot{m}_c \times c_p \times (T_{max} - T_5)] \tag{3.7c}
\]

The amount of fuel relative to the air supplied is then only about 1/30, which is small enough to be neglected. We can simplify EQ 3.7a, then, as:

\[
\dot{Q}_H = [\dot{m}_c \times c_p \times (T_{max} - T_5)] \tag{3.7d}
\]

In doing so, only \( T_{max} \) needs to be specified as a parameter, and the model user is free to set \( T_{max} \) as an independent parameter. Even if mass loss is included in the model, as it is in Section 3.8, absolute results may be off due to the simplification in EQ 3.7c, but the model is enhanced by its ability to do direct comparative analysis based on maximum temperature rather than fuel input rate. Calculating A/F and equivalence ratio for a given \( T_{max} \) and fuel type is a subject for future modeling work on the PACE engine.

3.5 The PACE Expander—Adiabatic Expansion with Pressure Losses

The expander processes are quite similar thermodynamically to the compressor's, except in reverse. These are depicted in Fig. 3.5 Consequently, the equations for pressure loss are the same. The light
Fig. 3.5 -- PACE Expander p-V Diagram
line $f'\rightarrow g'\rightarrow h'\rightarrow i'\rightarrow f'$ is the ideal or isentropic process; $f\rightarrow g\rightarrow h\rightarrow i\rightarrow f$ is the modeled process; and $f\rightarrow g'\rightarrow h'\rightarrow i''$ represents an actual expander cycle.

When the expander piston reaches TDC at $f$ the inlet valve opens and the new gas charge begins to enter, mixing with residual gases left in the clearance volume. The gases from the combustor at $p_6$ enter the expander cylinder at $p_7$ and continue to be forced into the space until the expander reaches volume $V_7$ (the "intake" volume at $g$), at which point the inlet valve closes.

Since full expansion is assumed in the expander design, the RPM of the expander differs from that of the compressor in order to accommodate the total mass flow and still reach full expansion. Once the working fluid stops entering (at $V_7$), the confined gas will expand to ambient pressure (line $g\rightarrow h$). Section 3.10 deals with the problem of full expansion using a variable volume expander (VVE) rather than a variable speed drive (VSD).

A certain amount of excess work will be expended in discharging the expander gas ($h\rightarrow i$). The height of the pressure "hump" depends upon the engine speed and port geometry. After the piston returns to TDC, only a small amount of high-temperature, residual gas will be left in the clearance volume, and the cycle begins again.

In this model the residual gases are recompressed along line $i\rightarrow f$. The advantage of recompressing the gas is to ensure that the pressure differential across the intake port is minimized to avoid the effects of the pressure shock when gas velocities exceed sonic speed. It may well be that the degree of recompression assumed in this model may not be
necessary, but this would need further empirical and analytic investigation.

Note that in Fig. 3.5 the expansion line ends at point h which is some pressure, \( p_g \), above the exhaust (ambient) pressure. As it turns out, full expansion to ambient pressure, then some recompression to drive out the exhaust gases requires more work than the loss in availability incurred by using some blowdown to accomplish the same purpose. In this model the pressure difference \( (p_g - p_9) \) is exactly the pressure difference calculated by EQ 3.5.

3.6 Inclusion of Heat Transfer in PACE Compressor and Expander Components

Heat transfer is treated as a total quantity for both the compressor and expander using EQ 2.14, the overall heat transfer equation adapted from Taylor [12]. The heat transfer calculation is, at best, an estimate, but one well-founded on first principles.

In this model all viscosity and conductivity values are for those of air at the appropriate temperature, \( T_g \). Although this assumption may appear arbitrary and would be incorrect for working fluids other than air (particularly combustion gases), it must be kept in mind that the greatest source of error is in determining an accurate value for \( T_g \). By assuming air as a working fluid and using air properties, the model can perform air standard analysis. Then all parametric runs are based on consistent working fluid properties. \( T_g \) is determined as a weighted average of temperatures calculated on a cycle basis for the compressor
and expander processes. Accurate values for $T_g$ need to be determined empirically.

Note also that the value for $K$, the overall heat transfer constant, is regime-specific. $K$ would be different for the compressor than for the expander. It must also be determined empirically. If one uses the value of $K$ equal to 10.4 (a dimensionless coefficient), which applies to IC engines [12], then heat losses from the PACE expander would range upwards beyond 50% of the adiabatic work, which is unacceptable and probably not reasonable. In Chapter 5, a way to estimate a value for this coefficient is proposed. Just how the coefficient, $K$, would change if ceramic materials were to be used is not clear and would have to be addressed experimentally.

Taylor [12] also suggests that, although EQ 2.17 is valid for a wide range of $T_g$ and for both four- and two-stroke engines, the equation is not strongly influenced by either the thickness of the cylinder walls or the material conductivity. Keep in mind that Taylor's data is derived from engines composed of aluminum, cast iron, and steel materials, which have high conductivity. In comparing the heat transfer characteristics of all these samples, the dominant factor is the Reynolds number of the working fluid, which really determines the heat transfer coefficient, $h_e$, by giving large weight to the forced convective effects on the inside of the cylinder.

The effects of using different cylinder materials, however, could be accommodated by adjusting the coefficient, $K$, in EQ 2.13. Subsuming the effects of low-conductivity, high temperature-tolerant ceramics into the overall heat transfer equation, EQ 2.13, as just described, may be
an oversimplification. But it does allow a modeler to make comparisons among different materials by using a different coefficient, $K$, for each material type. Furthermore, it should be remembered that material conductivity has a strong effect on the value of $T_g$ since a conductive cylinder wall will draw heat out, and diminish the gas temperature, while a ceramic material, being non-conductive, will keep heat in and the temperature up. Higher temperatures will also tend to increase the temperature gradient, thereby encouraging heat transfer even more than at lower temperatures. The net effect of increased temperature with lower conductive materials may not mean a large reduction in relative heat transfer rates. Whether this is true remains to be determined experimentally.

3.7 Friction Coefficient and the Rate of Friction Work in the Compressor and Expander

Friction is easily treated as a linear function of average piston speed. It is also treated as a load which the piston must counter, and therefore does not affect enthalpy of the working fluid during the expander or compressor work cycle (see assumption 5, Section 3.1). Friction does, however, have a dramatic effect on efficiency, net specific work, and power. As described in Chapter 2, the friction coefficient, $f$, is used to determine a mean effective pressure ($fmep$), over a cycle, for the work done to overcome friction.

$$fmep = f \times u$$  \[3.9\]

and
\[ W_f = (A_p * u) * \frac{f_{mep}}{2} \]  

where \( W_f \) is the rate of friction work, and \( A_p \) is the piston face area, \( u \) is average piston speed, and division by 2 is for the number of strokes per cycle. As noted earlier, pressure effects are not accommodated and realistic values for \( f \) are not available without conducting further experiments on the PACE compressor and expander. The friction coefficient accounts for all mechanical friction including the friction of the piston rings as well as all mechanical linkages associated with the component, whether the expander or compressor. A way to estimate the PACE friction coefficient is presented in Chapter 5.

3.8 Inclusion of Mass Loss in Compressor and Expander

When cylinder valves are closed, and the working fluid in a cylinder is contained under positive pressure during compression or expansion, there will be some mass loss. However, mass loss through leakage around piston rings and valve seats is generally limited to a few percent in typical piston devices. For the purposes of this model, only mass lost during compressor compression and residual gas reexpansion and during expander expansion will be considered. Mass lost during recompression of residual gases at the end of the expander exhaust stroke is not analyzed because it does not affect expander mass flow rate calculations. All the model requires is that the pressure in the expander at the end of recompression be adjusted to equal the average intake pressure \( (p_f) \). In effect, the mass processed by the expander is independent of the amount of mass lost in recompression.
Decher [13] proposes mass loss to be a linear relationship of both pressure ratio and piston speed. His theoretical framework is more detailed than is necessary for this parametric model. What is important is that a parameter must be derived which accounts for a reasonable reduction in total mass as pressure increases and speed decreases. The faster the average piston speed, u, and the smaller the ratio of ambient to cylinder pressure in the cylinder, \( p_0/p \), the lower the mass loss rate. As a first approximation, then, we can introduce a mass loss parameter, \( \beta \), which decreases linearly with higher pressure ratio and lower piston speed:

\[
\beta = \left(\frac{u}{u_{\text{max}}} \right) \left( \frac{p_0}{p} \right)
\]

where \( p_0 \) is ambient pressure and \( u_{\text{max}} \) is the maximum piston speed (3000 ft/min). Note that when \( u \) is very small, or if \( p \) is very large, the mass loss effect is most pronounced and \( \beta \) tends toward zero. However, as \( \beta \) tends toward unity, then the mass loss is minimized. EQ 3.11 is constrained to vary from zero to unity, where \( 0 < \beta < 1 \).

So far, all this mass loss parameter does is provide a basis to account for mass loss as a linear function of pressure ratio and average piston speed. An actual equation which can be used in the model must still be developed.

The discussion which follows focusses on the compression process, but applies equally well to the expansion process. At this point an important assumption is made about modeling the processes of compression and expansion in a closed cylinder. Recall that the working fluid is modeled as being compressed isentropically when no mass is lost. Since
the amount of mass lost during a compression (or expansion stroke), is very small (on the order of less than 5%) we assume the working fluid left in the cylinder is also compressed isentropically. The implication is that the thermodynamic properties of the reduced amount of working fluid at the end of compression are isentropic, or the same as if there were no mass loss.

The isentropic expressions relating temperature, pressure and volume apply here:

\[
\frac{p}{p_0} \sigma = \left(\frac{V_0}{V}\right)^{y-1} = \frac{T}{T_0}
\]

where \( \sigma \) is \( [(y - 1)/y] \). Only mass and volume need to be calculated to compare the isentropic/no-mass-loss case to the isentropic/mass-loss case. Figs. 3.6A and 3.6B show profiles of compression and expansion. In both cases, \( V_y \) designates the actual volume with mass loss, and \( V_x \) the volume without mass loss. The calculation of mass left in the cylinder after compression is as follows:

\[ M_x = \frac{pV}{RT} \]
\[ M_y = \frac{pV}{RT} \]

End pressure is a given, and the gas constant, \( R \), is the same in both equations. Temperature can be determined from the isentropic equation given in EQ 3.12. Since \( T_x = T_y \), based on the one assumption made above, the question remains, how does one calculate \( V_x \) and \( V_y \)? EQs 3.13a and 3.13b can be combined in this way:

\[ \frac{M_x}{M_y} = \left(\frac{V_x}{V_y}\right) \]
Fig. 3.6A -- Mass Loss and the Modified Polytropic Exponent for Compression

Fig. 3.6B -- Mass Loss and the Modified Polytropic Exponent for Expansion
We can make use of a modified polytropic exponent, \( n \), to try to resolve this. To determine a thermodynamic state, the properties of the working fluid at that state are independent of the process used to arrive at it. For an isentropic compression, the process can be characterized by EQ 3.1. Since \( V_y < V_x \) we might use a polytropic path, where \( pV^n \) is constant, to determine the value of \( V_y \) -- if an appropriate value for the exponent, \( n \), can be found. For the isentropic process with a small amount of mass loss, we propose to use a modified polytropic expression:

\[
    n = 1 + (V - 1) \ast (1 - \lambda)
\]  

[3.14]

where \( \lambda \) is a value less than unity. Here in EQ 3.14, the mass loss parameter, \( \beta \), already introduced, shows up. But the mass loss factor, \( \lambda \), needs some explanation.

In effect, as long as \( \lambda \) equals unity, the modified polytropic exponent, \( n \), reduces to the isentropic exponent. In this case there is no mass loss effect. However, if \( \lambda \) is less than unity, then \( 1 < n < V \). As it turns out in the model analysis if \( .95 < \lambda < 1 \), then the mass loss is less than 5\% over a wide range of pressure ratios and piston speeds and this approach to modeling mass loss seems to work quite well.

Now, volumes can be calculated:

\[
    V_y = (p_0/p)^{1/n} \ast V_0 \tag{3.15a}
\]

\[
    V_x = (p_0/p)^{1/V} \ast V_0 \tag{3.15b}
\]
The ratio $M_y/M_x$ is the proportion of mass left in the cylinder, and $Y$ is the mass lost.

$$M_y/M_x = (p_0/p)^{1/n - 1/Y}$$  \[3.16\]

and

$$Y = 1 - M_y/M_x$$  \[3.17\]

3.9 Equations for the PACE Engine System Model

The First Law of Thermodynamics analysis is the basis for the PACE model developed in this thesis. For an open system, with steady flow, the governing energy balance equation is [21]:

$$\dot{m} \times (h_o - h_i) = \dot{W} - \dot{Q}$$  \[3.18\]

where the sign convention is positive for any work done on the system and negative for any heat leaving the system. The kinetic energy terms are not included because the relative difference between the inlet and outlet mass flows is assumed to be negligible. The subscripts $i$ and $o$ are for in and out, respectively. Looking back to the compressor and expander diagrams (Figs. 3.2 and 3.3), we develop the First Law as it applies to these two components.

3.9.1 Compressor Work

The compressor, like the expander, is modeled as a two-part system. The first component is adiabatic, as discussed in Section 3.3,
and EQ 3.18 becomes:

\[ \dot{W}_C' = m \cdot (h_4 - h_0) \]  \[3.19\]

where the prime denotes adiabatic work. But, the actual rate of work (or power) can be expressed as follows:

\[ \dot{W}_C = m \cdot (h_5 - h_0) + \dot{Q}_C \]  \[3.20\]

We must first calculate the net additional amount of power used by the compressor in the actual versus the adiabatic case. To determine \( \Delta \dot{W} \), the additional work rate input required because of heat loss from the compressor, we take the difference between EQ 3.19 and EQ 3.20:

\[ \Delta \dot{W} = m \cdot (h_5 - h_4) + \dot{Q}_C \]  \[3.21\]

Next, a value for \( T_5 \) in Fig. 3.2, the exit temperature from the compressor, must still be determined. The heat transfer rate, \( \dot{Q}_C \), is calculated using EQ 2.14, based on the assumptions and conditions discussed in Section 3.6. Using the following relationship, it is clear that if a value as large as \( c_p \) were used for the coefficient, \( C \), it would negate the heat transfer component if plugged back into EQ 3.21:

\[ \dot{Q}_C = m \cdot C \cdot (T_4 - T_5) \]  \[3.22\]

As a maximum, \( C \) must be less than \( c_p \), but large enough to get a significant temperature difference \( (T_4 - T_5) \) where \( T_5 < T_4 \). If we arbitrarily choose the constant volume specific heat, \( c_v \), this will provide a consistent reference for all working fluids and be a readily
determined parameter for the model. It is also always less than the constant pressure specific heat value, which is what we are looking for.

\[ \dot{Q}_C = \dot{m} \cdot c_v \cdot (T_4 - T_5) \]  \[3.22a\]

Substituting EQ 3.22a back into EQ 3.21, the following relationship is derived:

\[ \Delta \dot{W} = \dot{m} \cdot [(h_5 - h_4) + c_v(T_4 - T_5)] \]  \[3.23\]

Adding this incremental amount of power to the adiabatic component of EQ 3.19, we get:

\[ \dot{W}_C = \dot{m} \cdot [(h_4 - h_0) + (c_v - c_p)(T_4 - T_5)] \]  \[3.24\]

Simplifying, assuming constant specific heats for a perfect gas:

\[ \dot{W}_C = \dot{m} \cdot [c_p(T_5 - T_0) + c_v(T_4 - T_5)] \]  \[3.25\]

3.9.2 Expander Work, Net Specific Work, and Engine Thermal Efficiency

The analysis of the expander model proceeds in the same way. First, looking at both the adiabatic component and the definition of actual rate of work:

\[ \dot{W}_E' = \dot{m} \cdot (h_6 - h_9) \]  \[3.26\]

But, the actual power out can be expressed as follows:

\[ \dot{W}_E = \dot{m} \cdot (h_6 - h_{10}) - \dot{Q}_E \]  \[3.27\]
To determine $\Delta \dot{W}$, we take the difference between EQs 3.26 and 3.27:

$$\Delta \dot{W} = \dot{m} \cdot (h_g - h_{10}) - \dot{Q}_E$$  \[3.28\]

Using the same assumption for heat transfer in the expander as used in the compressor:

$$\dot{Q}_E = \dot{m} \cdot c_v \cdot (T_9 - T_{10})$$  \[3.29\]

where $T_{10} < T_9$.

And, finally, substituting EQ 3.29 back into EQ 3.28, the following relationship is derived:

$$\dot{W} = \dot{m} \cdot (c_v - c_p) \cdot (T_9 - T_{10})$$  \[3.30\]

And EQ 3.30 becomes:

$$\dot{W}_E = \dot{m} \cdot [c_p(T_6 - T_9) + (c_p - c_v)(T_9 - T_{10})]$$  \[3.31\]

Finally, we are in a position to determine an expression for net specific work and overall engine thermal efficiency. Using EQs 3.31 and 3.25, combined with the expression for the rate of friction work, EQ 3.12, net power and net specific work are determined:

$$\dot{W}_{net} = \dot{W}_E - (\dot{W}_C + \dot{W}_{f(E)} + \dot{W}_{f(C)})$$  \[3.32\]

$$w = \frac{\dot{W}_{net}}{\dot{m}}$$  \[3.33\]
Lastly, using EQ 3.32 and EQ 3.7d the calculation of engine thermal efficiency is defined like this:

\[ e_t = \frac{\dot{W}_{\text{net}}}{\dot{Q}_H} \]  \[3.34\]

### 3.9.3 Estimation of Component Efficiencies

Adiabatic efficiency and component efficiencies were discussed in Section 2.7. In trying to determine a component efficiency value for the PACE compressor or expander, an "ideal" rate of work must first be known.

For the compressor, the ideal work rate is generally taken to be the isentropic work per cycle of compressing a mass charge from ambient pressure up to the prescribed pressure ratio.

\[ \dot{W}_{C(\text{ideal})} = \dot{m} c_p T_0 ( R_c \sigma - 1) \] \[3.35\]

where \( \sigma = (\gamma - 1)/\gamma \).

The mass flow rate, \( \dot{m} \), in this relation cannot be determined without accounting for the effects of pressure losses and heat transfer which influence volumetric efficiency to a large extent. Also, the average specific heat must be known, which means actual time-dependent temperature profiles must be tracked to get a weighted average value for \( c_p \). Furthermore, EQ 3.35 uses a nominal pressure ratio, but the actual pressure ratio may not be quite the same. The exit pressure from the compressor after discharge does not quite equal the nominal pressure in the model due to pressure losses at the exit valves.
Calculated component efficiencies, therefore, are an approximation, and may even result in values slightly greater than unity when heat transfer and friction effects are minimized.

Combining EQ 3.35 with EQ 3.25, the equations for compressor component efficiency then becomes:

\[ e_C = \frac{m c_p T_0 (R_o^\sigma - 1)}{\dot{W}_C + \dot{W}_f(C)} \]  

[3.36]

where \( \dot{W}_C \) and \( \dot{W}_f(C) \) for the compressor are given by Eqs 3.25 and 3.12, respectively.

Similarly, an equation for the expander component efficiency can be expressed as:

\[ e_E = \frac{\dot{W}_E + \dot{W}_f(E)}{m c_p T_f (1 - (p_6/p_9)^{-\sigma})} \]  

[3.37]

The same limitations of the compressor equation also apply here, namely pressure ratio is a nominal value, \( c_p \) is a weighted average, and mass flow rate is actual, rather than ideal.

3.10 Variable Speed Drive (VSD), Variable Volume Expander (VVE), and Matching Compressor and Expander Components

Although the equations developed so far can be used for calculating engine performance, no means has been presented to match separate compressor and expander components. There are several governing criteria which must be satisfied if a compressor and expander are to be compatible.
As was explained in Section 3.5, the PACE expander must accommodate all the mass flow from the compressor and also reach full expansion volume—without over- or under-expansion. It must operate this way over a wide range of temperatures and pressure ratios and mass flow rates. Compressor cylinder bore and stroke can vary over a wide range, as can the number of cylinders as well as other design parameters. The same is true for the expander. How, then, can one fix the important design features of both components, especially physical dimensions, so that mass continuity and range of performance criteria are satisfied?

Both a variable speed drive (VSD) and a variable volume expander (VVE) have been suggested by Decher [9] as ways to deal with this. Fig. 3.7 illustrates this problem. In a VSD, $V_{E'}$, the expander stroke volume, $V_E$, is fixed, and the expander RPM operates independently of the RPM of the compressor. For the VVE, the RPM of expander and compressor are the same, while the expander volume, $V_E$, can be designed to vary over some range (maybe as much as 2 to 1) to match mass flow rate between compressor and expander.

The relation between RPM and expander volume, at any given mass flow rate is approximated by the following relationships:

$$\dot{m}_C = \dot{m}_E = \rho E * u * A_p \quad [3.38]$$

where $\rho$ is the density of the working fluid at the end of the expansion stroke, and $u$ is the average piston speed.

$$u * A_p = V_E * (RPM/60) * B \quad [3.39]$$
VE(min) -- VE(max)

OPERATING
REGION

\( V_E^* \)

\( V_E(min) \)

Increasing \( \dot{m} \)

Lines of constant mass flow

Maximum Mass Flow Line

RPM* (expander)

\( \dot{m}_1, \dot{m}_2, \dot{m}_3, \dot{m}_4, \dot{m}_5 \)

Fig. 3.7 -- Expander Operating Points
In EQ 3.38, we may assume expander density to be constant over a range of RPM for a given flow rate. This means volumetric inefficiencies are insignificant, which is the case at low speeds and high valve-to-piston area ratios. Therefore, the quantity \( \left( V_E \cdot \text{RPM} \right) \) on the right side of EQ 3.39 is a constant, and lines of constant density/constant mass flow rates can be plotted as hyperbolic curves, as illustrated in Fig. 3.7. Here, \( V_E \) is on the ordinate and \( \text{RPM}_E \) on the abscissa. The interesting thing about this curve is that it portrays all operating points for an expander, whether the design is a variable speed drive or a variable volume expander. The heavy line e-e is the line of maximum mass flow, \( \dot{m}_{E}^\text{max} \), the expander can accommodate. Any higher mass flow rate would require either a larger \( V_E \) or a faster RPM, both of which are beyond the design limits.

A variable volume expander, operating at a constant RPM, can operate anywhere between the two volumes \( V_E(\text{max}) \) and \( V_E(\text{min}) \) at a corresponding RPM for a given mass flow rate. For a VVE the bore is fixed, but the stroke varies, and \( V_E \) is proportional to the stroke. The larger \( V_E \), the longer the stroke and the faster the average piston speed at a given RPM. Piston speed (see EQ 2.5) is constrained to a maximum of 50 ft/sec. Since \( \text{RPM}_{\text{max}} \) is inversely proportional to the stroke, a larger \( V_E \) (longer stroke) means a slower \( \text{RPM}_{\text{max}} \). Similarly, a variable speed drive expander operates at a fixed \( V_E \) and can accommodate a maximum mass flow indicated by the line e-e.

An example will demonstrate the greater flexibility one has in using a VSD rather than a VVE design. Suppose \( \text{RPM}^\text{*} \) is the operating RPM for a VVE design. Then between \( V_E(\text{max}) \) and \( V_E(\text{min}) \) the operating line
crosses only one constant mass flow line, c-c. In contrast, if $V_E^*$ is the design stroke volume for a VSD, then the operating line crosses every constant mass line a-a, b-b, c-c, d-d, and e-e on the diagram since RPM can vary over a wide range. For this reason, the analysis conducted with the PACE software model in Chapter 5 of this thesis focuses exclusively on a VSD design.

Finally, this brings us to the question of component matching of compressor and expander in the PACE engine. The one real constraint in defining one's choice of expander to be paired with a particular compressor, or vice versa, is the principle of mass continuity. The expander chosen must accommodate the mass flow rate of the compressor. Ideally, one would like the matched pair to operate over a broad range of RPM. The easiest way to assure this, especially in selecting the expander to match the compressor, is to use a VSD. Then the expander RPM can vary independently of the compressor and a wide range of mass flow rate can be accommodated.

However, if one chooses a VVE, then one is constrained to operate over a very narrow mass flow range as described in the example above. Perhaps the only reason one would choose a VVE over a VSD is cheaper cost or the unavailability of a suitable VSD coupling. Whether the PACE design is based on a VSD or VVE, the objective is to eliminate the excessive blowdown the expander would experience if the exhaust gases could not reach full expansion to ambient pressure. Either a VVE or VSD would solve this problem, or a combination of both.

Almost any-sized expander could be matched with a particular compressor, as long as the compressor could deliver the pressure and
mass flow required. There may be a design configuration combination of the expander and compressor which operates in a range where power, efficiency, and net specific work in combination are optimized. Also, there may be some combination of VSD and VVE design which is best, depending on what the design or performance criteria might be. If this were the case, one would have to develop a control algorithm which would determine the optimum RPM\textsubscript{E} and V\textsubscript{E} combinations over the range of performance for a particular compressor/expander configuration. Nevertheless, matching an expander to fit the characteristics of a compressor requires careful analysis. Optimum strategies to address this are beyond the scope of this thesis.

3.11 Applications of a Parametric Analysis Model

In the development of any analytic model, an important question is, "Does the model accurately analyze the performance of the actual engine it is supposed to represent?" In the case of the PACE engine, there is no actual operating engine one can use to validate model results. But, we have identified the key parameters and established critical assumptions needed to develop a reasonable model. The basic approach used here has been to derive appropriate relationships from first principles and to adapt data borrowed from studies on engines that have similarities which match the PACE in many respects. In the case of the PACE engine, the model developed here uses information obtained from studies of other internal combustion engines, primarily spark ignition
and Diesel examples. There are some important differences, and these have been noted.

The best kind of model, if accuracy is the overriding criterion, is a time-dependent simulation. This kind of model performs an energy and mass balance for a finite number of time increments during a cycle, the smaller the crank angle, the more accurate the simulation. Such a model would use differential equations and complex matrix mathematics. A simulation model could accommodate transient conditions as well as steady state, and could be designed to deal with complex time-dependent input data. But such a model is way beyond the scope of this project. To begin with, the required input data are not even known for steady-state conditions. In addition to being cumbersome to develop algorithms for this kind of software, a simulation model could take orders of magnitude more time to run than a simplified, but reasonably accurate, and useful parametric analysis model.

A parametric model provides these key advantages:

a. Identifies important design and operating parameters which influence engine performance characteristics. These are treated as input data for the software model; this gives the model user full flexibility in analyzing any particular engine design.

b. Parameters can be tested, in groups or individually, to evaluate the relative effects these parameters have on overall engine performance.

c. Absolute accuracy of the model within very narrow tolerance cannot be assured, primarily due to the inherent inaccuracy or
uncertainty in basic assumptions and input data. The equations
describing the relationships and interactions among the
different parameters in this model are founded on basic
thermodynamic principles. However, the relative, or
comparative, differences resulting from the model's parametric
comparative analysis should be valid to a reasonable degree in
both magnitude and direction of the change.

The next chapter outlines the BASIC software model, followed by
the results of the parametric analysis reported in Chapter 5.
CHAPTER 4

SOFTWARE DEVELOPMENT

This chapter reviews the design of the software model--its development and its algorithms--in detail. The program is listed in Appendix B. Table 4.1, below, describes the model's structure.

<table>
<thead>
<tr>
<th>Applesoft BASIC Lines</th>
<th>Program Unit Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 - 999</td>
<td>INPUT</td>
</tr>
<tr>
<td>1000 - 4350</td>
<td>ANALYSIS and CALCULATIONS</td>
</tr>
<tr>
<td>4500 - 4620</td>
<td>OUTPUT</td>
</tr>
<tr>
<td>5000 - 9855</td>
<td>SUBROUTINES</td>
</tr>
</tbody>
</table>

**Detailed BASIC Description**

1 - 9
10 - 145
150 - 245
250 - 325
330 - 480
500 - 999
1000 - 1350
1700 - 1775
1900 - 2000
3500 - 3810
4010 - 4350
4500 - 4620

**SUBROUTINES**

5000 - 5320
5500 - 5790
9000 - 9020
9100 - 9240
9300 - 9380
9400 - 9855

variable speed drive RPM (VSD)
variable volume expander volume (VVE)
estimate sizing for expander
air viscosity and conductivity calculations
error messages
extra output
A flow chart of the basic model is depicted in Fig 4.1. This model is designed as a structured program. It has a top-down approach, composed of discrete subroutines and units, with the input, analysis, and output portions carefully separated and independent. There are no unconditional GOTOs, so the program flow can be followed in a linear fashion, and edited, if necessary, without destroying the program structure.

This model uses a line editor for input, rather than a menu-driven, "user friendly" approach. However, an IBM version of the model has been developed by Martin [23], and has extensive menus for input data, parametric analysis, and built-in graphics output. Martin has adapted this Apple model to the IBM PC which is more widely available and considered an industry standard.

4.1 Software and Hardware Specifications

The model was developed in Applesoft BASIC, using a DOS 3.3 disk operating system, on a 64K RAM Apple IIe microcomputer, with one disk drive designated in slot 6. An OEM 80-column card is required to produce full screen view for editing and output.

The graphics output is designed to be interfaced with an EPSON RX-80, or equivalent, using an Orange Micro Grappler+ printer interface card. The supplementary graphics software is the SCIENTIFIC PLOTTER™ purchased from Interactive Microware, of College Station, PA. The graphics package provides for X-Y data points input from files, the keyboard, or directly from user-defined subroutines. It has automatic
EDITOR (G.P.L.E.)

START

INPUT
* design characteristics (exp/comp)
* operation characteristics
* operating parameters
* working fluid properties

RUN-TIME ERRORS

ANALYSIS & CALCULATIONS

SUBROUTINES
* VVE or VSD
* error messages
* air properties
* select output

OUTPUT
* performance indices
* P, T

YES

RE_RUN PARAMETERS?

NO

STOP

SCREEN

OPTIONAL PLOTTER
scaling, can plot up to five curves per graph, then dump the graph to the screen, printer or data file.

The interactive editor used to revise parametric input is the G.P.L.E.™ from Beagle Bros. of San Diego, CA. For complete details, the reader is referred to manufacturers' documentation manuals for application of these software packages and Apple hardware.

4.2 Input

As was described in Chapter 3, the 38 input parameters have been divided into five main groups and these are listed in Table 4.2: compressor design characteristics, expander design characteristics, operation characteristics, and working fluid properties. Operating parameters are the compressor RPM, the maximum temperature (at expander inlet), the pressure ratio, and the variable volume multiplier when the model uses a variable volume expander (VVE). The choice of the Variable Speed Drive (VSD) or the VVE is a different "MODE" in the program (see line 380).

Design characteristics include bore, stroke, number of cylinders, cycles per revolution, mean flow coefficients (inlet and exit), and the piston-to-valve area ratios for both compressor and expander. These have been defined in the previous two chapters.

Operation characteristics are aspects of the engine operation which may be independent of compressor or expander design, or must be determined empirically: friction coefficients, overall heat transfer
### Table 4.2 — PACE Model Input Parameters

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Notes</th>
<th>Parameter Name</th>
<th>Units</th>
<th>Range (Notes)</th>
</tr>
</thead>
<tbody>
<tr>
<td>b</td>
<td>(1)</td>
<td>bore</td>
<td>inches</td>
<td>no restrictions, but $0.8 &lt; b/s &lt; 1.25$</td>
</tr>
<tr>
<td>s</td>
<td>(1)</td>
<td>stroke</td>
<td>inches</td>
<td>no restrictions, but $0.8 &lt; b/s &lt; 1.25$</td>
</tr>
<tr>
<td>$A_i$</td>
<td>(1)</td>
<td>piston/valve area ratio (inlet)</td>
<td>dimensionless</td>
<td>$1 &lt; A_i &lt; 20$; $5$ to $10$ common</td>
</tr>
<tr>
<td>$A_e$</td>
<td>(1)</td>
<td>piston/valve area ratio (exit)</td>
<td>dimensionless</td>
<td>$1 &lt; A_e &lt; 20$; $5$ to $10$ common</td>
</tr>
<tr>
<td>$C_i$</td>
<td>(1)</td>
<td>mean inlet flow coefficient</td>
<td>dimensionless</td>
<td>$0.3 &lt; C_i &lt; 0.8$; $1.0$ theoretical maximum</td>
</tr>
<tr>
<td>$C_e$</td>
<td>(1)</td>
<td>mean exit flow coefficient</td>
<td>dimensionless</td>
<td>$0.3 &lt; C_e &lt; 0.8$; $1.0$ theoretical maximum</td>
</tr>
<tr>
<td>$C_{Cv}$</td>
<td>(1)</td>
<td>clearance volume (% of swept volume)</td>
<td>%</td>
<td>no restrictions, but $0.8 &lt; b/s &lt; 1.25$</td>
</tr>
<tr>
<td>$B$</td>
<td>(1)</td>
<td>number of cycles per revolution</td>
<td>psi atm</td>
<td>depends on design gearing or cams; PACE I has $3$ design dependent</td>
</tr>
<tr>
<td>$N$</td>
<td>(1)</td>
<td>number of cylinders</td>
<td>psi atm</td>
<td>design dependent</td>
</tr>
<tr>
<td>$f$</td>
<td>(2)</td>
<td>friction coefficient</td>
<td>lbf-sec/ft$^2$</td>
<td>$0 &lt; f &lt; 10$; must be determined empirically</td>
</tr>
<tr>
<td>$K$</td>
<td>(2)</td>
<td>overall heat transfer coefficient</td>
<td>BTU/sec-ft$^2$-°F</td>
<td>$0.95 &lt; K &lt; 3$; $10.4$ for IC engines; regime-specific</td>
</tr>
<tr>
<td>$\alpha_h$</td>
<td>(2)</td>
<td>combustor (heater) efficiency</td>
<td>dimensionless</td>
<td>if $0.95 &lt; \alpha_h &lt; 1.0$, then mass loss is $&lt; 5$%</td>
</tr>
<tr>
<td>$\Delta P_1$</td>
<td>(2)</td>
<td>pressure drop at compressor inlet</td>
<td>psi</td>
<td>typical $0.75 &lt; e &lt; 0.95$</td>
</tr>
<tr>
<td>$\Delta P_2$</td>
<td>(2)</td>
<td>pressure drop across combustor</td>
<td>psi</td>
<td>$&lt; 5$ psi is reasonable</td>
</tr>
<tr>
<td>$\Delta P_3$</td>
<td>(2)</td>
<td>pressure drop across expander</td>
<td>psi</td>
<td>$&lt; 10%$ is reasonable</td>
</tr>
<tr>
<td>$c_p$</td>
<td>(3)</td>
<td>average constant pressure specific heat</td>
<td>BTU/ft$^3$-°F</td>
<td>$0.95 &lt; K &lt; 3$; $10.4$ for IC engines; regime-specific</td>
</tr>
<tr>
<td>$c_v$</td>
<td>(3)</td>
<td>average constant specific heat</td>
<td>BTU/ft$^3$-°F</td>
<td>$0.95 &lt; K &lt; 3$; $10.4$ for IC engines; regime-specific</td>
</tr>
<tr>
<td>$c_{p,0}$</td>
<td>(3)</td>
<td>average constant volume specific heat</td>
<td>BTU/ft$^3$-°F</td>
<td>$0.95 &lt; K &lt; 3$; $10.4$ for IC engines; regime-specific</td>
</tr>
<tr>
<td>$T_0$</td>
<td>(4)</td>
<td>ambient temperature</td>
<td>°F</td>
<td>no restrictions, but $T_0 &lt; 32^\circ F$</td>
</tr>
<tr>
<td>$P_0$</td>
<td>(4)</td>
<td>ambient pressure</td>
<td>psi</td>
<td>approximately atmospheric</td>
</tr>
<tr>
<td>RPM</td>
<td>(5)</td>
<td>pressure ratio (compressor)</td>
<td>rev/min</td>
<td>no restrictions except $v &lt; 3000$ ft/min</td>
</tr>
<tr>
<td>$T_e$</td>
<td>(5)</td>
<td>maximum temperature (at expander inlet)</td>
<td>°F</td>
<td>limited by material tolerance</td>
</tr>
<tr>
<td>$P_{max}$</td>
<td>(5)</td>
<td>maximum pressure ratio</td>
<td>dimensionless</td>
<td>limited by material tolerance</td>
</tr>
<tr>
<td>$X_v$</td>
<td>(5)</td>
<td>variable volume expander (VVE) multiplier</td>
<td>dimensionless</td>
<td>maximum $K_e$, dictated by clearance volume; see Eq 3.2a</td>
</tr>
<tr>
<td>MODE</td>
<td>(5)</td>
<td>VSD or VVE (one or the other)</td>
<td>--</td>
<td>depends on expander design configuration</td>
</tr>
</tbody>
</table>

**NOTES:**
1. This parameter applies to both expander and compressor (design characteristics).
2. This parameter applies to both expander and compressor (operation characteristics).
3. This parameter applies to compressor processes.
4. This parameter applies to processes after the compressor (combustor and expander).
5. This is one of three independent operating parameters.
factors, mass loss factors, combustor efficiency, and pressure drops across the combustor and at the compressor inlet.

The working fluid properties are specified and used as average values and they have a significant effect on overall engine performance. These are the specific heats (both constant volume and constant pressure) and the ambient pressure and temperature of air.

The user has complete flexibility in choosing any combination of all these inputs, within a reasonable range. There are no actual default values, but reasonable input values are listed in Table 4.2. Input values are changed from previous numbers for parametric runs by invoking the GPLE line editor, using CTRL-E. Once a value is changed, the user simply hits the RETURN key and the analysis proceeds.

The general approach an analyst would use starts first at specifying a particular engine design configuration. This would entail defining all the physical dimensions and design characteristics of both the compressor and expander components. Then, appropriate operation characteristics (friction and heat transfer factors, etc.) would be selected. Lastly, the independent operating parameters would be varied over a range to determine engine performance at specific operating points. An operating point is defined as the combination of pressure ratio, compressor RPM, and maximum temperature—the independent operating parameters—at which the engine operates.
In analyzing the engine performance, first the mass flow of the compressor is determined and the compressor exit pressure, taking into account pressure and mass losses and volumetric efficiency. Mass flow is critical because the model must determine the number of expander volumes and revolutions needed to accept, and process, all this mass to satisfy the principle of mass continuity. Clearly, compressor volumetric efficiency is important in determining this quantity. Inlet Mach index influences volumetric efficiency, as does clearance volume and pressure ratio. After mass flow rate is calculated, the model estimates compressor heat loss and then estimates compressor exit temperature and pressure, passing these values to the combustor. Maximum temperature and pressure drop are then calculated at the combustor.

The expander is constrained to reach full expansion, while using some blowdown to overcome pressure losses during exhaust. Depending on whether the user chooses a VVE of VSD, the algorithms for the expander analysis will be different. Note that the program determines the expander intake volume, \( V_7 \), by first calculating the required blowdown delta-\( p \) pressure and adding this on to the exhaust pressure, \( p_g \). Then, using the relationship of EQ. 3.1 the program backs into the value of \( V_7 \) by knowing \( p_7, p_8 \), and the expanded volume, \( V_8 \) (see Table 3.1 for state point subscripts).

For the VSD, the expander's swept volume is fixed, but the RPM varies independently of the compressor RPM. In this case, the expander
must accept hot gas of a certain density and flow rate from the combustor. The initial expansion volume, \( V_7 \), is predetermined since it must lie at the intersection of the expansion line and the intake pressure, \( p_7 \) (see Fig 3.5). Therefore, the RPM is adjusted up or down in the subroutine beginning on line 5000 to accommodate the total mass flow. This subroutine returns a value for the RPM at which the expander must operate.

If the user chooses a VVE instead, the RPM is fixed but the exact value of \( V_7 \) must be determined. The subroutine beginning on line 5500 returns the calculated value for the actual swept volume for the given conditions of RPM, mass flow rate, and pressure ratio.

Once the expander analysis is complete, the model calculates expander heat transfer, then calculates compressor and expander friction work, combustor heat input rate, net specific work, engine thermal efficiency, and power density.

The model detects errors when inconsistencies occur which are the result of incompatible input data. If for any reason, for example, the compressor and expander are mismatched in size, or not capable of performing under the conditions given (e.g. pressure ratio too high, excess maximum temperature, piston exceeding sonic speed, etc.), the model renders an error message. The user must rectify the design or operating problem indicated by the message before the model will give good results. Such problems as an undersized expander, a compressor or expander operating at too-high a speed, or heat transfer and friction factors which are too high will all cause error messages to appear on the screen.
4.4 Output

The basic engine performance output consists of a listing of the three performance indices discussed earlier: efficiency, net specific work, and power density. The user has the option to print more information, such as compressor and expander RPM, volumetric efficiency, admission coefficient and so on. The user can also take advantage of the graphics software and prepare standard plots. However, one must keep in mind that this model is an interactive one, and requires a lot of user testing to examine the bounds and range of engine performance before a reasonable set of points can be determined to be valid for plotting.

4.5 Model Debugging, Testing, and Validation

Like all software models, the PACE program is prone to bugs, and many were discovered—and subsequently fixed—in the course of developing and applying the model.

As far as debugging the model, though, very deliberate steps were taken to test all the subroutines and algorithms in the software. Each subroutine was developed and tested independently. This has ensured that the values for the variables returned from the subroutines could be cross checked by hand calculations over a broad range of data output possibilities.

Aside from the usual bugs, like wrong subscripts in arrays or typos in variable names, the most difficult problems were encountered in the two expander subroutines: one for a variable volume expander (VVE),
and one for a variable speed drive (VSD). The problem in both cases was one of convergence.

The nature of this problem is that an exact expander RPM (for the VSD subroutine) and an exact expander swept volume (for the VVE subroutine) must be determined to provide mass conservation between the compressor and expander. RPM and expander swept volume are found by an iterative algorithm. An estimated value is guessed, initially, to be used to calculate an RPM or an expander swept volume which is somewhere between the maximum and minimum possible. The program performs a test to see how close the guess compares to a reference value by evaluating a residual difference between the two. If the residual difference is too large, a new estimated value is substituted by the program and then the maximum and minimum values are reset. The maximum and minimum values continue to be reset until the residual difference between them becomes relatively small compared to some reference difference.

The resolution of the model in iterating to an exact solution, given the reference difference, is about +/- 4% for the VSD subroutine, and about the same tolerance for the VVE routine. For example, for the VSD the calculated RPM of 2400 for the expander may be 100 RPM off the actual value of 2500. In the case of the VVE, the stroke volume may be calculated to be 4% larger than it actually is. To get better resolution would mean to narrow the residual difference described in the previous paragraph and require a lot more CPU time. It should be noted that the model tends to lose its accuracy at the extreme ends of the RPM scale. So the convergence error, although minor, is magnified, and points plotted near zero RPM and near RPM$_{\text{max}}$ should be avoided.
It was also difficult to account for all the possible error conditions one might encounter in trying to operate a particular engine design configuration outside reasonable operating limits. There are plenty of error messages and suggested solutions in the program to provide feedback for adjusting the model if this should be the case. Most run-time errors of this sort are due to trying to run the engine at operating points (maximum temperature, RPM, and pressure ratio) where the expander and compressor capacities do not match.

Fixing bugs, though, by itself, will not ensure that a model is useful or even accurate. The process of verifying the model's accuracy is called validation. In the case of the PACE, complete model validation will have to await the availability of empirical data. In the absence of such information, the "reasonable and comparable" criteria applies for validation purposes.

The comparable criteria indicates that the curve trends, overall shapes, relative peaks, and comparative profiles compare well to IC engine data reported in the literature. Power curves, pressure ratio parametric curves, and other plotted results, shown in Chapter 5, do, indeed, look similar to IC engine curves.

In the course of running the model, many calculated values were printed out and checked for reasonableness. Calculated efficiencies, for example, are what one might expect, and less than the maximum theoretical Brayton cycle efficiency for a given pressure ratio. Values of output variables were also checked to determine whether the trends in variable values were consistent with predicted behavior. In all cases where this test was applied, the data checked out fine. Mass loss,
component efficiencies, mass flow rates, thermodynamic state points, relative volume values—all checked out.
CHAPTER 5

RESULTS OF MODELING THE PACE ENGINE PERFORMANCE

Once the software model was debugged and tested to the extent possible, the next task was to complete a thorough evaluation of a PACE engine model by using the tested software. Model parameters were organized into discrete groups, segregating the input variables into logical associations as listed in Table 4.2 and described in Chapter 4. The PACE engine model has a total of 38 inputs which the user can specify. Table 4.2 specifies the nomenclature and symbols used for these variables. Table 4.2 also defines reasonable ranges for each variable, or a suitable reference where an appropriate value can be found. Mathematical relations or derivations upon which these variables are founded are discussed in Chapter 3.

All input data is arranged into five groups: operating parameters, compressor design characteristics, expander design characteristics, engine operation characteristics, and working fluid properties. In using the software one can take several approaches in analyzing a particular PACE engine design:

1. Development of an engine design configuration;
2. Performance analysis and the creation of an engine "map";
3. Sensitivity analysis of input parameters;
4. Comparative analysis of parametric performance curves; and
5. Evaluation of interactive and separate effects of parameter groups.
Each of these approaches is illustrated or described in this chapter. Note that the number of combinations of engine design configurations which could be evaluated using the PACE model is virtually unlimited. However, it is relatively easy to limit the combinations of input parameters for analysis to a few well-chosen groups of parameters which would thoroughly exercise the model's capabilities while demonstrating the kinds of analysis and results one can expect. In the discussion which follows the effects of all the input parameters are evaluated.

5.1 Development of an Engine Design Configuration

Although this model has tremendous analysis capability, it cannot design an engine. It will not select optimum bore/stroke ratios, clearance volumes, or other design characteristics for a compressor or expander. More importantly, it cannot match these two PACE components for optimum performance. Informed user choice and systematic analyses are required to optimize a particular design configuration. Optimum engine design depends critically on design performance criteria. Does the analyst want high power density, or maximum engine thermal efficiency? Over what pressure ratio and RPM range is the engine expected to operate? Once the model user has answered these questions, as well as defined some of the physical parameters of engine design (such as the number of compressor and expander cylinders in the engine housing), then engine performance can be analyzed and improved designs can be selected.
What the model can do is analyze a given engine's performance at specified operating conditions to determine how it will operate. For example, after specifying an engine design configuration, the user will input the three independent operating parameters: pressure ratio ($R_c$), compressor RPM ($RPM_c$), and maximum temperature ($T_{\text{max}}$). Then, after choosing operation characteristics and working fluid properties (see Table 4.2), the user can "run" the engine. The output—efficiency ($e_t$), net specific work ($w$), and power density ($P$)—will tell the user right away whether the engine performs to meet his or her expectations. The user can vary these three operating parameters over a reasonable range and see whether the engine operates satisfactorily over the range given, and how well it does perform.

If the engine cannot operate at some combination of these independent parameters, error messages appear. RPM running too fast, excessive pressure losses, and mismatch of compressor and expander are a few of the conditions which will trigger a simulation (run-time) error. These errors essentially say the engine cannot physically operate at the conditions prescribed. Based on this feedback information, the user can then adjust his engine design or input specifications in order to increase expander volume, change compressor stroke, try a larger piston/valve area ratio, or vary some other parameter to get the engine operating.

The steps to be followed in designing an engine would be as follows:

1. Determine the maximum and minimum values (range) for all three operating parameters ($R_c$, $RPM_c$, $T_{\text{max}}$).
2. Specify all the design characteristics of the compressor and expander, then the operation characteristics and working fluid properties.

3. "Run" the engine at the high and low ends of the operating parameters. Note any error messages which indicate why the engine, or compressor or expander components, cannot operate at the given extreme.

4. Adjust the component design characteristics or other parameters accordingly.

Using this approach, a particular engine design configuration was chosen as the reference model, or base case, for analysis in this chapter. The parameters selected are listed in the second column of Table 5.1, the base case values. All base case parameter values were selected as mid values over the range representing average values one might expect to use in modeling a PACE engine. Several literature sources as well as basic assumptions were used to estimate reasonable values of parameters as follows:

a. Specific heat values were taken from Fig. 11, p.732 of Obert [17]. For the compressor, 600°F was selected as the average gas temperature, whereas 1200°F was used for the expander.

b. Heat transfer coefficients, \( K_1 \) and \( K_2 \), are based on an estimated heat loss of 4% of compressor adiabatic work, and 15% for the expander, at \( \text{RPM}_c=2000, R_c=10 \) and \( T_{\text{max}}=1500°F \). See the discussion on heat transfer coefficient "calibration" below.
<table>
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<tr>
<th>PARAMETERS</th>
<th>PARAMETER RANGE</th>
<th>THERMAL EFFICIENCY</th>
<th>NET SPECIFIC WORK BTU/lbm</th>
<th>POWER DENSITY HP/cu.in.</th>
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</table>
c. Friction coefficients, $f_1$ and $f_2$, are determined similarly to the heat transfer coefficients. Using a value of $f_1=f_2=5$, results in a 12.3% loss in adiabatic work due to friction for the compressor and a 14.1% loss for the expander, at the specified operating conditions. See the discussion on heat transfer coefficient "calibration" below.

d. The mass loss factors chosen yield no more than about 3% mass loss at maximum pressure and minimum RPM.

e. The operating point used as the standard reference for sensitivity analysis and engine "calibration" (see discussion below) is given as 2000 RPM, $R_c=10$, and $T_{max}=1500^\circ F$. These are reasonable and comparable values to IC engines. Note that 2000 RPM, with the engine designed at 2 cycles per revolution, is equivalent to 4000 RPM for a four-stroke IC engine with one cycle every two revolutions. Also, the choice of $B=2$ cycles/rev is arbitrary and depends solely on the PACE engine's physical design.

f. The expander swept volume was matched to accommodate mass flow rate from the compressor at the indicated operating point. What this implies is that the compressor and expander are designed to run at approximately the same RPM (see Section 3.5 for further discussion on component matching).
The piston aspect ratio, bore/stroke (b/s), is unity. For most automotive pistons this aspect ratio ranges from about 0.8 to 1.25.

In the case of the heat transfer and friction coefficients, selection of the values given in items (b) and (c), above, is a way of "calibrating" the model, since no empirical data is available for narrowing these coefficients down to actual values for the PACE. This was done by estimating values for these parameters that would result in heat transfer and friction losses in both expander and compressor which were comparable to IC engines losses. For piston compressors, heat transfer accounts for about 5-15% of the adiabatic work, while this range is greater, about 10-35%, for IC engines. As for friction, f_mep is about 5-20% of the overall mep. Since mep is proportional to work, this information bounds the problem of trying to find a reasonable value for f. Lacking better information, we assume IC data is applicable to the PACE.

Performance curves for the base case engine design configuration are presented in Fig. 5.1. In this graph, the power density and efficiency curves show typical performance profiles compared to IC engines. The power density curve increases less than linearly with RPM, and starts to taper off as the parasitic losses become more pronounced at higher RPMs. But the efficiency curve reaches a maximum at about 600 RPM, then drops dramatically as the irreversibilities due to speed begin to take over. Heat transfer, in particular, increases more than
Fig. 5.1 -- PME Engine Performance Curves

Engine Thermal Efficiency

Net Specific Work (BTU/lbm)

Power Density (HP/cu.in.- Expander)
linearly at higher speeds, as do pressure losses, which increase with the square of engine speed.

The approach to engine design described in this section is clearly interactive and makes use of the model's parametric analysis capability. It is also very helpful in first determining whether a particular engine design configuration can actually operate at the extreme ends of the desired ranges of pressure ratio, compressor RPM, and maximum temperature. The next section describes the analysis and development of the engine performance which can be represented on an engine "map".

5.2. Performance Analysis and the Creation of an Engine "Map"

The procedure just described allows the user to test the extreme limits of an engine's performance capabilities, given minimum and maximum pressure ratio, RPM, and temperature combinations. By specifying both compressor and expander design characteristics, as well as the values for the engine operation characteristics and working fluid properties, an analyst can vary pressure ratio as a parameter with RPM as the independent variable. Then, the analyst can plot efficiency, net specific work, or power density as functions of compressor (or expander) RPM. Once the performance curves for each pressure ratio parameter are plotted, curves connecting constant values of net specific work or efficiency can be overlaid to complete the graph shown in Fig 5.2.

Note that this engine map represents performance for a single maximum temperature (1500°F) and for a particular engine design configuration.
Fig. 5.2 — PACE Engine Performance Map

- $w =$ net specific work
- $R_e =$ pressure ratio

- Operating Limit Line

Engine Thermal Efficiency

RPM
Fig 5.2 is an example of a performance map for the case of $T_{\text{max}} = 1500^\circ\text{F}$. Engine thermal efficiency is plotted against $\text{RPM}_c$, with pressure ratio, $R_c$, as a parameter, and with loci of constant net specific work connected across the pressure ratio parametric curves.

The engine map profile speaks for itself, but there are several features which merit discussion. First, in the lower right corner of the map, there is a "performance limit line". This line identifies the operating limits for the engine which are due, primarily, to insufficient expander capacity to accommodate the mass flow from the compressor. Generally, this means the expander is undersized for operating points to the right of this demarcation.

Clearly, the combination of optimum efficiency and net specific work lies around $R_c = 12$ and $\text{RPM}_c = 600$. Note also how the constant net specific work lines run approximately horizontal at low RPMs and lower pressure ratios but curve upward and back at higher pressure ratios and higher RPMs. This behavior may be associated with the crowding of the pressure ratio curves at the top of the map. The gains in efficiency as pressure ratio gets higher and higher become less and less, and the principle of diminishing returns manifests itself. This appears to be the case here.

However, there is more. If one can accept the results represented in Fig. 5.2, then it appears there may be a maximum operating pressure ratio. Note how the efficiency curve for $R_c = 25$ is lower than the curve for $R_c = 20$. The effects of diminishing returns aside, it could be that this anomaly may be attributed to the effects of heat transfer and pressure losses as they begin to dominate at higher pressure ratios. In
particular, the relative proportion of heat lost at higher pressure ratios may exact a higher efficiency penalty than is worth paying for.

5.3. Sensitivity Analysis of Input Parameters

One of the most valuable applications of this model is its ability to run sensitivity analyses on the several parameters which drive it. Three sets of graphs, Figs. 5.3, 5.4, and 5.5, present the results of a comprehensive sensitivity analysis of all the input parameters used in analyzing this particular engine design at the specified operating characteristics. Table 5.1 lists the base case values used in the analysis (the same as the engine design), the extreme values of the parameters (both high and low), and the results to three significant figures. These are the data plotted in Figs. 5.3, 5.4, and 5.5.

Figs. 5.3, 5.4, and 5.5 graphically show the sensitivity of engine thermal efficiency, net specific work, and power density, to relative changes in the model's input parameters. On each of these graphs, there lies a vertical line which represents the base case value for the performance index. There are four horizontal lines crossing these vertical axes. Each of the four lines shows sensitivity of the performance parameter to a set of parameters—compressor design characteristics, expander design characteristics, operation characteristics, and working fluid properties. All the parameter values above the parameter horizontal line are for increases to the base case values, and all parameter values below the horizontal are for decreases.
Fig. 5.3 -- Sensitivity Analysis, Effects of Parameter Changes on Engine Thermal Efficiency
Fig. 5.4 — Sensitivity Analysis, Effects of Parameter Changes on Net Specific Work
Fig. 5.5 -- Sensitivity Analysis, Effects of Parameter Changes on Power Density
Sensitivity analysis demonstrates which input parameters have the most significant effect on output values $e_t$, $w$, and $P$. The approach taken is described as follows:

1. Construct a base case engine design configuration and specify base case operation characteristics and working fluid properties (these are the middle column values in Table 5.1);

2. Choose high and low values of the parameters to coincide with reasonable extreme values of the parameters likely to be used as input values;

3. Put all differential changes in parametric values on the same relative scale in order to make comparisons among parameters;

4. Identify the parameters which have the most significant effect on increasing or decreasing engine performance indices.

An explanatory note is appropriate here. In doing the sensitivity analysis, the objective is to determine which parameters have the most significant effect on the performance indices (efficiency, net specific work, and power density). The incremental change in a parameter is the change from the mid-range value to the high and low range values for each parameter. This approach allows one to see the relative effects of each parameter change at the high and low range, or best and worst case. The alternative is to change each parameter by a fixed percent, then evaluate the effects. The shortcoming of that approach is that one ends up comparing apples and oranges. For instance, changing the combustor
efficiency by 10% would be appropriate, but changing the mass loss factor (which is really an exponential value) by 10% takes it right out of reasonable range.

Strictly speaking, the sensitivity analysis must be qualified if valid comparisons are to be made. Looking at Table 5.1, for example, one could say that doubling the friction coefficient of the expander has a greater effect on reducing efficiency than doubling the friction coefficient of the compressor. Or, increasing the piston/valve area ratio, $A_i$, of the expander has a more pronounced effect on efficiency than the same increase in the $A_i$ of the compressor. All comparisons would have to be made in a similar way: relative comparisons among similar parameters.

As for the operation characteristics, the most profound changes are indicated by the friction and heat transfer factors ($f$ and $K$) of the expander. Engine performance appears to be most sensitive to heat transfer and friction factors, so this only underscores the need to have good empirical data in order to establish model inputs. Without further experiments into the behavior of the PACE engine in these respects, input values for heat transfer and friction parameters are, at best, good "guestimates".

Small changes in specific heats, both for constant pressure and constant volume, also appear to be significant. One way to reduce the margin for error in user-specified $c_v$ and $c_p$ is to include algorithms within the model to calculate these parameters rather than have them user-specified. The problem here is that these values would require accurate temperature calculations, and temperature is linked to accurate
heat transfer calculations, which are perhaps the least reliable in the whole model. Furthermore, unless one were willing to limit the model to air standard analysis, one would have to accommodate equations for specific heats of a wide variety of gas constituents, particularly for exhaust gas compositions. Ultimately, this probably means a combustion model would need to be included. If this were the case, the run time required might become unwieldy and the advantages of a microcomputer model would be negated.

Results highlight the importance of valve design and operation, as represented by the mean flow coefficients ($C_i$ and $C_e$) and piston/valve area ratio ($A_i$ and $A_e$) parameters. One would expect that maximum valve area and maximum flow coefficient values would result in the best performance. This is, in fact, true, except for the compressor $C_i$ and $A_i$ where one sees the opposite effect with regard to efficiency and net specific work.

Less significant effects are indicated by the piston/valve area ratio parameters (both inlet and outlet, of compressor and expander) as well as the mean inlet and exit flow coefficients. What this indicates is that pressure losses have less influence on overall performance than friction and heat transfer losses. Neither mass loss effects nor pressure drop through the combustor are very significant. However, pressure drop at the compressor inlet can be significant. This means that engine derating would have to be considered at non-standard applications, such as at higher altitudes. Supercharging will also have a profound effect on thermodynamic performance.
Clearance volume is an important parameter, affecting all three performance indices. However, changes in expander clearance volume have the opposite effect of equal changes in compressor clearance volume, except for the effects these changes have on power density where these effects are quite dramatic. In considering the reason for these effects, it should be noted that the volumetric efficiency of the compressor is tied directly to clearance volume. Reducing the compressor clearance volume will enhance the volumetric efficiency which is proportional to power.

For the expander, the admission efficiency (as calculated using the admission coefficient, $\eta_a$) is independent of the expander clearance volume. What really matters is how the pressure drops are calculated at compressor admission and at the expander intake. The pressure drop during compressor admission influences volumetric efficiency probably more than clearance volume. Note also the relatively insignificant effect of changes in the ambient pressure parameter.

Both the compressor and the expander bores appear to influence strongly all three performance indices, but the effects are opposite for the compressor and expander. Whether one increases the compressor bore relative to the expander or vice-versa depends on which performance index is to be emphasized.

Overall, the relative effects of the compressor design and operation characteristics have less effect on engine performance than comparable changes in expander parameters. Since the compressor work rate is about 40-60% of the expander power output, it stands to reason
that the losses associated with the compressor would be proportionately less.

Investigating performance sensitivity to small changes in parametric values is a very straightforward and simple, but powerful, analysis procedure. The one serious limitation to this approach is that the results are only valid for the operating point defined (in this case \( \text{RPM}_c = 2000, \ R_c = 10, \ \text{and} \ \text{T}_{\text{max}} = 1500^\circ\text{F} \)). Interactive effects among parameters may cause differing results at different ranges of the operating parameters. However, the direction of change in performance due to an increase or decrease in a parameter would likely remain the same for most parameters. Just the relative effect of one parameter compared to another may change in magnitude. Ideally, one would first develop a performance map of a proposed engine design, determine the operating point most desired, then run the sensitivity analysis to confirm which design or operation characteristics need to be developed to improve performance.

5.4 Comparative Analysis of Parametric Performance Curves

Another approach one can use to assess the relative effects of various parameters is to actually vary a specific parameter over the operating range (\( \text{RPM}_c \) and \( R_c \)) of the engine and compare how parametric curves differ. Figs. 5.6 through 5.10 are some examples of how parametric curves may be plotted. Fig. 5.6 shows efficiency and power density versus \( \text{RPM}_c \) with \( \text{T}_{\text{max}} \) as the parameter. The truncated lines for \( \text{T}_{\text{max}} \) of 2000\(^\circ\text{F} \) and 2500\(^\circ\text{F} \) are due to insufficient expander capacity to
Fig. 5.6 -- The Influence of Temperature on Power Density and Engine Thermal Efficiency

(NOTE: Truncated curves indicate performance limit of this particular PACE engine design with this parameter).
operate beyond the points indicated. Note also the tendency for the curves to dip faster toward the x-axis as $T_{\text{max}}$ decreases, and the maximum power density shifts to the right as $T_{\text{max}}$ increases. What is most interesting is the lack of performance advantage at the higher temperatures. This may well be due to heat transfer effects. If this were the reason, then it depends critically upon the value of the heat transfer factor assumed in the engine model input.

Fig. 5.7 plots engine efficiency versus RPM$_C$ with expander heat transfer coefficient, $K_2$, as a parameter. Note that the maximum efficiency appears to shift to the left as $K_2$ decreases. Fig. 5.8 plots engine efficiency versus RPM$_C$ with expander friction coefficient, $f_2$, as a parameter. Again, the maximum efficiency appears to shift to the left as $f_2$ decreases, while the far right portion of the curves tend to level out as $T_{\text{max}}$ gets larger.

Figs. 5.9 and 5.10 show efficiency and power density as functions of RPM$_C$, with the clearance volume fraction of both expander and compressor as parameters. Clearly, the smaller the fraction for the expander, the better the efficiency. However, for the compressor this is not the case. At 1200 RPM the two compressor curves cross. At less than RPM = 1200 it appears that a higher clearance volume fraction for the compressor will produce better overall efficiency.

These few curves are a small sample of the kind of parametric analysis one could perform to investigate the relative effects of varying parameters. Other important parameters one might want to analyze in evaluating a particular engine configuration's performance are: piston/value area ratios, mean inlet and outlet flow coefficients,
Fig. 5.7 --- Effect of Expander Overall Heat Transfer Coefficient on Engine Thermal Efficiency
Fig. 5.8 -- Effect of Expander Friction Coefficient on Engine Thermal Efficiency
Fig. 5.10 -- Influence of Clearance Volume on Power Density

(NOTE: Truncated curves indicate performance limitations of the PACE engine design operating at the given parameter).
Fig. 5.9 - Influence of Clearance Volume on Engine Thermal Efficiency and Power Density

(NOTE: Truncated lines indicate engine performance limits for this design, given the specified parameter.)
and inlet pressure and temperature. In cases where comparing parametric curves tend to indicate constant proportional differences (a linear relation) the results will not be very interesting (see Fig. 5.11, for example). It is where parametric curves manifest different peaks, cross-overs, or unusual shapes that the analysis becomes most interesting.

5.5 Interactive and Separate Parametric Effects

One interesting analysis approach is to take groups of parameters and test them, one group at a time, to investigate their relative effects. Then once the largest parametric effects have been determined, the parametric groups can be run in sequence to see their interactive effects as shown in Fig. 5.11, which was developed using the base case parameter values in Table 5.1. Here, the maximum Brayton cycle efficiency is 0.482. A constant drop in efficiency, down to 0.435, is represented by adding a combustor efficiency, $e_H$, of 0.90. Next, all the parameters which affect pressure losses are incorporated—the mean flow coefficients, the piston/valve area ratios, and the combustor and compressor drops. Then the heat transfer coefficients are added. Lastly, the friction coefficients are included.

What is clear from this interactive composite profile is that pressure and friction losses increase dramatically as speed increases, but heat transfer losses are greatest at low speed.
Brayton Cycle, Maximum at $R_C = 10$

Efficiency with Constant Combustor Losses, $e_H = 0.90$

- with pressure losses
- adding heat transfer
- including friction

**Fig. 5.11 -- Interactive Effects of Various Parametric Groups on Engine Thermal Efficiency**
5.6 Scale Effects

In scaling the PACE engine up from its nominal 15 HP size represented by the base case engine, there are three ways to change the power output: increase displacement, increase RPM, or increase the number of cylinders. The base case model could just as easily have been done on an engine with twice as many cubic inches, more cylinders, or at higher RPM, and the nominal power rating would have been higher.

One might argue that a comprehensive analysis of one engine configuration cannot possibly cover the gamut of engine performance capabilities from a small 1 HP engine all the way up to 500 HP, which is the operating range for other IC engines. However, there are several key points to keep in mind about the relative effects of the model parameters which are likely to be significant as engine scale varies.

As far as increasing displacement, the critical parameters are the bore and stroke of both the compressor and the expander. However, the effects of these parameters can be compared by examining the influence of the piston aspect ratio, b/s. This ratio ranges from about 0.8 to 1.25. If the aspect ratio remains about constant as the piston is scaled up, the changes in bore and stroke will not significantly alter performance results (efficiency, net specific work, and power density). Power will, of course, scale up nearly proportion to displacement because the mass flow rate increases in almost direct proportion to displacement. The main factor which changes when the b/s ratio changes is heat transfer, which is affected primarily by bore. Because volume displacement increases with the square of the bore, the heat loss
increase is almost compensated for by the net increase in power. If the stroke change is large relative to the bore, then all speed effects will be more pronounced.

As for number of cylinders (N) and cycles per revolution (B), these parameters are linearly related to power and RPM, respectively. In this model, multiplying the number of cylinders will multiply the power proportionately and not affect efficiency or net specific work. Changing the value of B for a component will only affect the RPM (of compressor or expander) in direct inverse proportion. In other words, the performance indicated at, say, 2000 RPM with B=2, is the same as that at 4000 RPM, B=1, or 1000 RPM with B=4. Both RPM and cycles per revolution are directly related to average piston speed, u. Again, B is determined by the gearing arrangement in the PACE design.

On the other hand, the relative number of cylinders and cycles per revolution (B and N) for the compressor compared to the expander may make a significant difference. Since the relative work of the compressor is only a portion of the work output of the expander, all irreversibilities due to B and N differences between the compressor and expander should be less important when associated with the compressor rather than vice-versa.

By modeling a representative engine of four cylinders and two cycles per revolution, as done here, the resulting analysis should apply just as well to larger power output engines of more cylinders which have values of N and B that are multiples of the base engine configuration. As far as this model works, scale effects will not be significant unless piston aspect ratio changes. However, Fig. 5.12 shows that the effect
Fig. 5.12 -- Piston Aspect Ratio Effect on Engine Thermal Efficiency

Engine Thermal Efficiency

RPMc

b/s = 1.0

b/s = 1.25

b/s = 0.80
on efficiency over the range of \(0.8 < b/s < 1.25\) is not very significant when the aspect ratio change applies to both compressor and expander.

One should also bear in mind that the PACE engine is not limited to low horsepower as demonstrated in this analysis. Piston displacement (bore and stroke) and number of cylinders are entirely open-ended design parameters, and power can be scaled upward accordingly. In case of the PACE engine, though, power density should be carefully considered in proposing engine applications. For example, a Chevrolet Malibu 8-cylinder, 305 cu.in. engine is rated at 145 HP at 4000 RPM. The bore and stroke are 3.736 and 3.480, respectively, and the compression ratio is 8.6:1. This is a power density rating of 0.475 HP/cu.in. Now, a PACE engine of similar expander displacement — 8-cylinders, same bore, stroke, compression ratio (equivalent pressure ratio), and operating at 2000 RPM (same number of power cycles per min as the Chevy) at a maximum temperature of 1500°F — only achieves about 30 HP and a power density of 0.10. The critical difference between the two engines is, first, air density and mass flow rate, then pressure-temperature profile. The PACE may not reach comparable power densities of common IC engines, but this might be compensated for by better thermal efficiency at higher average operating temperatures.

There is one irreversibility which is probably not constant even if the piston aspect ratio remains constant—friction. The empirical values for the friction factor are probably strongly correlated to total cylinder surface area (circumference of the cylinder) and air density (pressure ratio). Although friction mean effective pressure (fmep) is
linear for a particular engine configuration, the friction coefficient is bound to vary with different engine designs.

While, friction effects due to scale are not accounted for in the model, the piston aspect ratio should still affect the friction coefficient. But empirical values related to scale effects are not available for making these comparisons without further experimental data.

Finally, the bore/stroke ratio does not appear to significantly affect engine performance so long as both compressor and expander piston aspect ratios vary the same. However, it appears efficiency and net specific work can be enhanced by minimizing the compressor piston aspect ratio while maximizing this ratio for the expander.
A microcomputer model has been developed which predicts the thermodynamic performance of a Brayton cycle engine with reciprocating piston compressor and expander components. The model is based on an air-standard open Brayton cycle without regeneration.

The model incorporates all important irreversibilities which include: heat transfer, pressure losses, mass loss and recirculation, and mechanical friction. Each irreversibility is modeled as a function of pressure ratio or average piston speed, which in turn is a linear function of RPM. Key independent operating parameters are maximum temperature, compressor RPM, and pressure ratio. Other input parameters are divided into four groups which include design characteristics of both the compressor and expander, parameters which characterize the irreversibilities, and properties of the working fluid. There are a total of thirty-eight input parameters.

Both a variable speed drive (VSD) coupling between the compressor and expander and a variable volume expander (VVE) are design options for the modeler. The modeler selects one or the other. The VSD design was exercised extensively in the analyses because it is more flexible in operating over a broad range of RPMs and pressure ratios compared to the VVE design. Both the VSD and the VVE are used to allow the expander to
reach full expansion to near-ambient exhaust pressure, thus avoiding the
inefficiencies associated with over- or under-expansion.

In this thesis, applicable data from research on IC engines have
been adapted to PACE engine designs. Data from studies on heat
transfer, friction, and pressure losses, in particular, have been used.
Certain parameters appear to influence PACE engine performance very
strongly, yet IC data for the PACE engine based on these values may not
be applicable to the PACE engine. The most critical parameters, notably
friction and heat transfer coefficients, must be determined
experimentally if accurate model results are to be expected. This
underscores the need to obtain good empirical data to validate the PACE
model.

Despite these limitations, the model has some innovative features.
It is interactive and sensitivity analysis is easily performed. The
model is a very powerful tool for comparing the influences of different
parameters and analyzing PACE components and engine design
configurations.

The model resolves the key processes in the compressor
(induction/compression/discharge/reexpansion) and in the expander
(intake/expansion/exhaust/recompression) and analyzes the
irreversibilities for each of these processes.

The PACE model is a powerful interactive tool for comparative
analysis and developing insight into the interactive effects of key
operating and design parameters. One can easily ask questions like, "If
the heat transfer coefficient were half as much, what would be the
resulting effect on engine efficiency, net specific work, or power
density?" This kind of sensitivity analysis is easy to perform with this model, and can serve as the foundation for comparing different engine configurations. Once the key parameters which influence engine performance are tested, improved engine designs can be developed, at least, in principle. Good empirical data for parameters which may have a dramatic effect in swaying engine performance are critical to the development of optimum engine designs.

This model can be applied in several ways. Key uses of the model are:

a. Preliminary Design of Engines -- PACE engines can be designed by interactively testing input data which defines component design and operation characteristics of the compressor, expander, and combustor. The model will tell the user whether the engine can operate at a given maximum temperature, pressure ratio, and RPM (an operating point). In other words, the model helps determine which components are compatible and can predict performance given a set of input parameters.

b. Comparative Analysis of Engine Designs -- By varying only one parameter at a time, or a group of parameters, the user can determine which parameters have the most critical effect on engine performance.

c. Sensitivity Analysis -- Relative effects of all parameters can be compared over the range of parameter input values expected to apply in the model. One can also group parameters and test
the effects of different groups, successively and separately, on engine performance.

d. Development of Engine "Maps" -- The model can be used to develop enough data points to create an engine map, showing the relationships among pressure ratio, efficiency, net specific work, and engine speed (RPM) for any given engine design configuration, given a maximum temperature and a specified set of operation characteristics.

e. Parametric Performance Curves -- A user can develop a set of comparative curves for any input parameter, overlay these upon a graph of one of the three performance indices versus engine speed. Any interesting trends or differences among these curves would be worth noting and may warrant further investigation. This approach was used in an extensive sensitivity analysis performed for single engine design.

As presented here, the PACE engine microcomputer model has demonstrated itself to be very useful for evaluating the effects of different input parameters on three engine performance indices: efficiency, net specific work, and power density. The emphasis in using the model is on relative comparisons rather than absolute accuracy in results. The reason for this is simple: a model is only as good as its least accurate assumption. As with all analytic models, absolute or accurate results can only be assured if the model assumptions are valid and the input data, itself, is accurate. Nevertheless, this work is the
first step in developing a comprehensive model to analyze the thermodynamic performance of the PACE engine as a complete system.
CHAPTER 7

RECOMMENDATIONS

There is the opportunity to analyze many more design configurations of the PACE engine than presented here. Recommendations offered here as a result of completing this thesis include: additional analysis or further research to narrow uncertainty in values for model parameters; improvements in model methodology and algorithms; and enhancement of model software and hardware.

7.1 Additional Analysis and Research

a. Sensitivity analysis -- The results presented in this report deal with a comprehensive sensitivity analysis of a base case engine model at a specific operating point. It would be useful to carry this approach further and determine the sensitivity of engine performance to various parameters at different operating points ($R_c$, $T_{\text{max}}$, $\text{RPM}_C$) to see how relative effects might vary at different operating points.

b. Component matching and component efficiencies -- The PACE compressor and expander need to be matched to satisfy certain design or performance criteria, most notably mass continuity. The expander must accept all the mass the compressor delivers, while still getting full expansion out of the piston. If compressor and expander maps were available for a range of component sizes and designs, a user could
decide which two components to put together to satisfy the mass continuity criterion while meeting other design criteria. These criteria might include meeting overall power density requirements while still achieving a certain efficiency level over a given RPM range. Only a particular combination of compressors and expanders might fit the bill.

**c. Variable volume expander** — Although the user has a choice of variable speed drive or variable volume expander, only the variable speed drive option was thoroughly tested. The variable volume expander has limited use, by itself, since the range of expander volume will only allow operation over a narrow range of RPM while still accommodating compressor mass flow (see Section 3.10). A variable volume expander (VVE) would be mechanically more complex, and would not be necessary to achieve both mass continuity and full expander expansion if a variable speed drive were used in the PACE engine.

**d. Comparison to other IC engines** — One interesting follow-on study would be a comparison of the differences and similarities of the PACE engine with other IC engines. Preliminary results from this analysis suggest that power densities for the PACE, for example, may be much less than for other IC engines given the same displacement volume of the PACE expander compared to an IC engine. Other aspects of performance should prove just as interesting.

**e. Optimization strategy** — This model does not optimize an engine design. But it does allow for iterative evaluation of various
parameters or groups of parameters. One can determine engine operating performance given a set of design and operation characteristics. Efficiency seems a likely performance index to try to optimize since net specific work appears to follow the efficiency profile, except at high RPMs. A good strategy would separate the important design and operation parameters and limit the investigation to a few parameters which can be controlled.

7.2 Model Improvements

There are a number of ways this basic model could be improved. Listed below, in order of expected importance, is a description of possibilities. Some of these are suggested, more appropriately, as questions which need to be answered:

a. Heat transfer -- Of all the irreversibilities, this one has the least analytic definition. If one were to continue to use the model as it now stands, better ways to estimate the heat transfer parameter (K), the mean effective gas temperature ($T_g$), and the overall effects of material conductivity would be the first order of business. If these could be improved, then functionally linking the specific heat values ($c_p$ and $c_v$) to actual temperatures would become possible and would improve model accuracy.

Alternately, modeling heat transfer as heat stored, then imparted to the working fluid on a cyclic basis may be a more realistic approach, and eliminate the need to estimate actual working fluid temperature leaving the cylinder, as is now done in this model. However, this
method not only requires input of thermal diffusivity values but also empirical determination of certain temperatures at certain points within the compressor or expander. Estimating these temperatures may not build any more accuracy in the model than is already there.

Keep in mind, air properties are used in the model to determine both viscosity and air conductivity. Having built-in table values for typical combustion gas compositions would also improve accuracy.

b. Friction -- Further investigation to determine realistic values of the friction coefficient is needed. Are the coefficients different for the compressor and the expander? Is there a functional relation between the bore to stroke ratio which might be incorporated into the model? Would mechanical friction (fmep) be significantly less for the PACE with sleeve valves versus IC engines with cam linkages?

c. Pressure losses and valve design -- Determination of actual values for the mean flow coefficients is critical. These values may differ for inlet and exit ports for both the compressor and expander and may also be speed dependent to some degree. This needs to be investigated further. Furthermore, the model uses a constant coefficient of 1.25, which is independent of piston speed, in pressure loss calculations. This is an oversimplification; the functional relationships which define this coefficient warrant further study.

d. Combustor modeling, intercooling, and recuperator, and supercharging -- This model does not model combustion processes. This aspect of a PACE engine can be dealt with separately, and does not have
a strong bearing on the analysis of the critical components—the reciprocating compressor and expander. Nevertheless, combustion efficiency could be modeled to broaden the model's capability. One would have to program the model to accept a variety of fuel and combustion gas properties, including air/fuel ratio, specific heats, and fuel heating values.

Efficiencies of any Brayton cycle engine can be enhanced using supercharging, intercooling in multistage compressors, and a recuperator to recover the heat in the exhaust. These also could be added to the model.

7.3 Software and Hardware Enhancements

At the time this project was conceived, the best available computer resource was the Apple IIe with Applesoft BASIC. There are newer, state-of-art versions of BASIC now which are less cumbersome to work with and lend themselves to better interfacing with output devices, especially plotters, rather than dot matrix plots. Newer MS DOS versions of BASIC provide direct graphing commands, structured BASIC routines, and compilers to make programs run faster and make debugging and programming more efficient and versatile. Alternately, other languages might be applied such as Pascal, FORTRAN, or C to take advantage of built-in compilers, structured programming features, or graphics plotting routines not available with Applesoft or other BASICS.

In addition to software improvements, one might take advantage of hardware enhancements for direct interface with high-resolution pen
plotters. There is always room for improvement with software and hardware, especially since the technology is advancing so rapidly. Development of a good computer software model, by its nature, is an evolving, never-ending kind of project.

One point, hopefully, remains clear throughout this analysis: the steady state operation of the PACE engine is tremendously complex. This model is a first attempt to try to identify all the important parameters affecting the engine's performance and to define the problem of constructing a realistic model of an operating PACE engine. In trying to make the model manageable, there has been a trade-off, sacrificing some detail and precision for ease of use. A higher degree of complexity and accuracy would only be possible with additional empirical data and by using intensive simulation modeling techniques. But, this model has the ability to resolve discrete effects of more parameters than originally expected, and it does so quickly with interactive ease. A complex simulation model would not be useful for this purpose.

The model has bounded the problem of how to analyze PACE engine performance. It requires some user sophistication to define reasonable input values to run a realistic model. As such, this model becomes the foundation of all the work yet to come, showing the potential of the PACE engine, a novel idea whose time has come.
REFERENCES


APPENDICES
APPENDIX A

DERIVATION OF VOLUMETRIC EFFICIENCY AND THE ADMISSION COEFFICIENT FOR THE PACE COMPRESSOR AND EXPANDER

PART I -- Volumetric Efficiency of the Compressor

Volumetric efficiency is the ratio of the amount of mass processed per cycle compared to the ideal amount. In the discussion which follows we refer to Fig. 3.4, the PACE Compressor p-V Diagram.

\[ e_v = \frac{M_{\text{actual}}}{M_{\text{ideal}}} \]

\[ e_v = \frac{(p_2(V_2 - V_1))}{(p_0 V_c)} \]

In regarding Fig. 3.4, we use the pressure at which the inlet valves open, \( p_1 \), as a basis for the analysis. Later, a correction is made to adjust the denominator used in the ensuing analysis to convert it to the "ideal" mass as defined in the equation above (see also line 1330 of the BASIC program in Appendix B).

First we define volumetric efficiency. We begin with an energy balance, taken directly from Taylor's appendix four [12].

The governing equation is:

\[ (M_i + M_r)E_2 - M_iE_i - M_rE_r = Q - w/J \]

where \( M_i \) is the mass of fresh air entering the cylinder;
Mr is the mass of the residual gases in the cylinder; 
w is the net work produced during the induction process; 
E is the internal energy per unit mass; and 
Q is the net heat received.

Now, the following relations hold:

\[ M_i = \rho_i V_d e_v \]
\[ M_r = \rho_r V_1 \]
\[ (M_r + M_i) = \rho_2 V_2 \]

Note that \( V_d = (V_2 - V_1) \), which is the induction volume, 
and the inlet condition is the same as state point 1 in Fig. 3.4. The 
net work involves both the pdV work in moving the piston as well as 
the flow work of moving the working fluid (air) into the cylinder. 
The \( \Delta T \) of the heat transfer is treated as if the entire fresh charge, 
\( M_i \), absorbs heat at a constant pressure during the induction 
process, so:

\[ w = - (\rho_i V_d e_v) + \int_{1}^{2} pdV \]
\[ Q = M_1 c_p \Delta T \]

Also,

\[ E = c_v T \]
\[ \rho = \rho/RT \]

Substituting into the energy equation:

\[ \left[ (V_2 \rho_2) - (V_d \rho_i e_v) - (V_1 \rho_1) \right] c_v/R = \int_{1}^{2} (\rho_i V_d e_v c_p \Delta T) + (e_v V_d \rho_i)/J - (1/J) \int_{1}^{2} pdV \]
Rearranging:

\[(V_2 P_2) - (V_1 P_1) = (V_d P_i e_v) + \frac{2}{R/Jc} \left[ (P_i V_d e_v c_p \Delta T/J) + (e_v V_d P_i) - \int_{1}^{2} p dV \right] \]

Since \( R/Jc = (k - 1) \) for a perfect gas, where \( k = \gamma = c_p/c_v \), substituting, then dividing through by \( (V_d P_i) \), and letting

\[ a = \int_{1}^{2} p dV/(V_d P_i) \]

\[ P_i = p_i/RT_i \]

\[ ((V_2 P_2) - (V_1 P_1))/(V_d P_i) = e_v + (k-1)(e_v - a) + (k e_v \Delta T/T_i) \]

Rearranging,

\[ e_v = ((V_2 P_2) - (V_1 P_1))/(V_d P_i) + (k-1)a \]

\[ k (1 + \Delta T/T_i) \]

Substituting \( r = (V_d + V_i)/V_i \), \( p_i = p_1 \), and letting \( \Delta T = 0 \) (adiabatic, as modeled), where \( a = p_2/p_1 \) we get:

\[ e_v = ((k-1)/k)a + [(a r - 1)/(k(r - 1))] \]

Noting that \( e_v \) holds for the inlet conditions and treats \( V_d \) as the swept volume, since \( M_{ideal} \) is actually based on a swept volume of \( V_c \):

\[ e'_v = e_v (V_2 - V_1)/V_c \]

And this is the equation used in the BASIC program, line 1330.
Part 2 -- Admission Coefficient for the PACE Expander

The admission coefficient is defined similar to the volumetric efficiency, and refers to Fig. 3.5:

\[ n_a = \frac{M_{\text{actual}}}{M_{\text{ideal}}} \]

\[ M_{\text{ideal}} = \rho_6 \left( V_{g^1} - V_{cv} \right) \]

\[ M_{\text{actual}} = \rho_7 \left( V_I - V_{cv} \right) \]

\[ V_{g^1} = V_8 \left( \frac{p_g}{p_6} \right)^{1/\gamma} \quad \text{and} \]

\[ V_I = V_8 \left( \frac{p_8}{p_7} \right)^{1/\gamma} \]

Substituting back we get:

\[ n_a = \frac{\rho_7 \left( V_I - V_{cv} \right)}{\rho_6 \left( V_{g^1} - V_{cv} \right)} \]
APPENDIX B

PACE SOFTWARE MODEL SOURCE CODE IN APPLESOFT BASIC
SPEED=255

JLIST

1 REM *** PACE ENGINE MODEL ***
2 REM *** BY TOM WHITE, M.S. THESIS ***
3 REM *** FOR DR. GEORGE TSONGAS, PROFESSOR OF MECHANICAL ***
4 REM *** ENGINEERING, PORTLAND STATE UNIVERSITY ***
5 REM *** NOVEMBER 1987 ***
6 REM
7 REM
10 REM ***----------------------------------***
20 REM *** INPUT ***
30 REM ***----------------------------------***
70 6 = 32.17: REM ** LBF/SEC^2 (GRAVITY)
80 J = 778.26: REM ** FT-LBF/BTU
90 PI = 3.14159
100 UMAX = .5: REM ** MAX PISTON SPEED, FT/SEC
110 PO = 144 + 14.1: P9 = PO: REM ** AMBIENT PRESSURE
120 CP(1) = .255:CP(2) = .270: REM ** SPECIFIC HEAT (CONST PRESS)
130 CV(1) = .505:CV(2) = .200: REM ** SPECIFIC HEAT (CONST VOL)
140 TO = 59 + 460:TI = TO:T2 = T1: REM ** INLET TEMPERATURES
150 REM
160 AC(1) = 5:AC(2) = 5: REM ** PISTON/VALVE AREA (COMP)
170 AE(1) = 5:AE(2) = 5: REM ** PISTON/VALVE AREA (EXP)
180 DIAM(1) = 2.5:STROKE(1) = 2.5: REM ** BORE/STROKE, COMPRESSOR
190 DIAM(2) = 3.00:STROKE(2) = 3.00: REM ** BORE/STROKE, EXPANDER
200 CLRVL(1) = .05:CLRVL(2) = .05: REM ** CLEARANCE VOLUMES
210 CI(1) = .6:CI(2) = .6: REM ** MEAN INLET FLOW COEFFICIENTS
220 CE(1) = .6:CE(2) = .6: REM ** MEAN EXIT FLOW COEFFICIENTS
230 B(1) = 2:B(2) = 2: REM ** CYCLES PER REVOLUTION
240 CYLINDER(1) = 4:CYLINDER(2) = 4: REM ** CYLINDERS PER REVOLUTION
245 REM
250 REM-----------------------------------
260 DP(1) = 1: REM ** PRESS DROP, COMP INLET (PSIA)
270 DP(2) = 2: REM ** PRESS DROP, COMBUSTOR (PSIA)
280 LAMBDA(1) = .99:LAMBDA(2) = .99: REM ** FLOW FACTOR
290 EFFICIENCY = .90: REM ** COMBUSTOR (HEATER) EFFIC.
300 DTRANS(1) = 1:DTRANS(2) = .25: REM ** HEAT TRANSFER FACTOR, K
320 FRICTN(1) = 5:FRICTN(2) = 5: REM ** FRICTION FMEP COEFFICIENT
325 REM
330 REM-----------------------------------
340 T6 = 1940: REM ** MAX TEMPERATURE
350 RC = 10: REM ** PRESSURE RATIO
360 VARVL = 1.20: REM ** VARIABLE VOLUME MULTIPLE
370 RPM(1) = 2000: REM ** COMPRESSOR RPM
380 MODE = 1: REM ** (1) VAR SPEED: (2) VAR VOL
390 TESTS = "YES": REM ** STATE POINT OUTPUTS (F,T)
400 K(1) = CP(1) / CV(1):K(2) = CP(2) / CV(2): REM ** RAD SPECIFIC HEAT
410 R(1) = (CP(1) - CV(1)) / K(1):R(2) = (CP(2) - CV(2)) / K(2): REM ** GAS CONSTANT
420 REM
500 REM-----------------------------------
510 DATA 1.483,2.671,3.481,5.46,7.57: REM VISCOSITY (KG/M-SEC * 10^-6)
520 DATA 250,500,750,1500,2500: REM PRESSURE IN BAR
530 DATA .009246,.04038,.117,.175: REM CONDUCTIVITY OF AIR
540 DATA 100,500,1900,2500: REM AIR TEMPERATURE FOR CONDUCTIVITY
550 READ MU(1),MU(2),MU(3),MU(4),MU(5)
560 READ TNU(1),TNU(2),TNU(3),TNU(4),TNU(5)
570 READ KAPPA(1),KAPPA(2),KAPPA(3),KAPPA(4)
580 READ TKAPPA(1),TKAPPA(2),TKAPPA(3),TKAPPA(4)
600 GOSUB 9000: REM DETERMINE SIZING FOR EXPANDER
999 REM
1000 REM ************************************************************
1010 REM *** COMPRESSOR ***
1020 REM *************************************************************
1040 RPMMAX = UMAX * 360 / (STROKE(1) * B(1))
1050 IF RPM(1) > RPMMAX THEN PRINT "COMPRESSOR RPM TOO FAST": END
1060 U(1) = STROKE(1) * RPM(1) * B(1) / 360
1070 VC = PI * ((DIM(1) / 12) ^ 2 / 4) * STROKE(1) / 12: REM **SWEPT VOLUME
1080 CLRVL(1) = CLRVL(1) * VC
1085 IF RC > (CLRVL(1) / VC) / CLRVL(1) * K(1) THEN PRINT "CLEARANCE VOLUME IS TOO LARGE OR ELSE PRESSURE RATIO IS TOO HIGH": END
1090 P3 = RC + PO
1100 Pl = PO - DP(1) + 144
1110 SIGMA(1) = (K(1) - 1) / K(1)
1120 T2 = T1
1130 T3 = T1 + RC * SIGMA(1)
1140 T4 = T3
1150 CMACH(2) = SQRT(K(1) * E + R(1) * T3)
1160 ZC(2) = AC(2) * U(1) / (CI(2) + CMACH(2))
1170 IF ZC(2) > .59442191 THEN GOSUB 9350
1180 P4 = P3 / (1 - .125 * ZC(2) - 2)
1190 Y1 = (U1) / UMAX * (Pl / P4)
1200 N(1) = 1 + (K(1) - 1) * Y1 * (1 - LAMBDA(1))
1210 VC = CLRVL(1) * (P4 / Pl) * (1 / N(I))
1220 CMACH(1) = SDR(K(1) - E + R(1) * T1)
1230 ZC(1) = AC(1) * U(1) / (CI(1) + CMACH(1))
1240 IF ZC(1) > .59442191 THEN GOSUB 9340
1250 P2 = Pl / (1 - .125 * ZC(1) - 2)
1260 V2 = VC * CLRVL(1)
1270 V3 = V2 + (P4 / P3) * (1 / N(I))
1280 RVOL(1) = V2 / VI
1290 IF V2 < VI THEN GOSUB 9380
1300 ALPH(1) = P2 / Pl
1310 DENSITY(1) = Pl / (R(1) * T1)
1320 MBSLOSS(1) = 1 - (P2 / P3) * (1 / N(I) - 1 / K(I))
1330 EV(1) = (K(1) - 1) * (RVOL(1) - 1) * ALPH(1) * ALPH(1) * RVOL(1) - 1) / (K(1) * (RVOL(1) - 1)) + ((V2 - VI) / VC)
1340 MC = (EV(1) * DENSITY(1) * VC + B(1) * RPM(1) / 60) * (1 - MBSLOSS(1)): REM MASS FLOW RATE PER CYLINDER
1350 REM
1700 REM ******************************************************
1705 REM *** COMPRESSOR HEAT TRANSFER CALCULATIONS ***
1710 REM ******************************************************
1720 TE(1) = (1 / (2 + VC)) * (((T2 + T3) / 2) * (V2 - V3) + T2 * (V3 - CLRVL(1)) + ((T4 + T1) / 2) * (V1 - CLRVL(1)) + T1 + (V2 - VI)) - 460
1721 T = (TE(1) - 32) * 5 / 9 + 273.16: REM DEG F TO DEG K
1722 GOSUB 9100: REM CALCULATE VISCOSITY AND AIR CONDUCTIVITY
1725 VS = VSITY(1) = VISCITY * 1 + 5
1727 CDUCTIV(1) = KAPPA
1730 AP(1) = ((DIM(1) / 12) - 2) * Pl / 4
1735 RE(1) = ((MC + DIAM(1) / 12) / AP(1)) / VISCOSITY(1)
1745 H(1) = (CNDCUVTIC(1) / (DIAM(1) / 12)) + STRANSFER(1) + RE(1) ^ .75
1755 DL(1) = AP(1) * CYLINDER(1) * H(1) * (TG(1) - 180)
1760 T5 = T4 - GL(1) / (MC * CV(1))
1770 P5 = P4
1775 REM
1900 REM ***-----------------------------------------------***
1910 REM *** EXPANDER ***
1915 REM ***-----------------------------------------------***
1925 RPM(2) = RPM(1)
1930 P6 = P4 * (1 - DP(2) / 100)
1935 VE = P1 * (((DIAM(2) / 12) ^ 2) / 4) + STROKE(2) / 12: REM ***SWEPT VOLUME
1940 VSMALL = VE
1945 CLRVL(2) = CLRVL(2) * VE
1950 VMA1 = VE + VVARVL
1955 VB = VE + CLRVL(2)
1960 RPMMAX = VMA1 * 360 / (STROKE(2) * H(2))
1965 IF ((MODE = 2) AND (RPM(2) > RPMMAX)) THEN PRINT "COMPRESSOR RPM TOO FAST": END
1970 IF MODE = 1 THEN GOSUB 5000
1975 IF MODE = 2 THEN GOSUB 5500
1976 V9 = CLRVL(2) + (P7 / P9) ^ (1 / (K(2)))
1978 VX = VB + (P8 / P6) ^ (1 / (K(2)))
1979 RHD7 = P7 / (R(2) * T7)
1980 DENSITY(2) = P6 / (R(2) * T6)
1985 EV(2) = (RHD7 * (V7 - CLRVL(2))) / (DENSITY(2) * (VX - CLRVL(2)))
1987 MASSLOSS(2) = 1 - (P8 / P7) ^ (1 / (N(2) - 1 / K(2)))
1990 ME = EV(2) * DENSITY(2) * (VX - CLRVL(2)) * BI(2) * (RPM(2) / 60) * (1 - MASSLOSS(2)): REM MASS FLOW RATE PER CYLINDER
2000 REM
3500 REM ***-----------------------------------------------***
3520 REM *** EXPANDER HEAT TRANSFER CALCULATIONS ***
3530 REM ***-----------------------------------------------***
3545 SIGMA(2) = (K(2) - 1) / (K(2))
3550 TB = T7 + (P7 / P8) ^ SIGMA(2)
3560 T9 = TB
3570 TB(2) = (1 / (2 * VE)) * (((T7 + T8) / 2) * (VE - V7) + T6 * (V7 - CLRVL(2))) + ((T7 + T9) / 2) * (V9 - CLRVL(2)) + T8 * (V8 - V9)) - 460
3577 T = (T6(2) - 32) / 5 + 273.16: REM DEG F TO DEG K
3578 GOSUB 9100: REM CALCULATE VISCOSITY AND AIR CONDUCTIVITY
3579 VISCOSITY(2) = VISCOSITY * 1E - 5
3580 AP(2) = (DIAM(2) / 12) ^ 2 + PI / 4
3585 CNDCUVTIC(2) = KAPPA
3590 RE(2) = (ME + DIAM(2) / 12) / AP(2) / VISCOSITY(2)
3630 H(2) = (CNDCUVTIC(2) / (DIAM(2) / 12)) + STRANSFER(2) + RE(2) ^ .75
3771 DL(2) = AP(2) * CYLINDER(2) * H(2) * (TB(2) - 180)
3800 TLAST = T9 - DL(2) / (ME + CV(2))
3810 REM
4010 REM ***-----------------------------------------------***
4020 REM *** CALCULATIONS ***
4030 REM ***-----------------------------------------------***
4050 WC = (MC / (1 - MASSLOSS(1) / 2)) + CYLINDER(1) * (CP(1) * (T5 - T0) + CV(1)) * (T4 - T5))
4060 FMEP(1) = FRICTN(1) + U(1)
4070 WF(1) = FMEP(1) * AP(1) * CYLINDER(1) * U(1) / (2 * J)
4100 FMEP(2) = FRICTN(2) + U(2)
4115 WF(2) = FMEP(2) * AP(2) * CYLINDER(2) * U(2) / (2 * J)
4120 WE = (ME / (1 - MASSLOSS/2) / 2)) * CYLINDER(2) * (CP(2) * (T6 - T9) - (CP(2) - CP(2)) * (T9 - TLAST))
4170 WNET = WE - WC - WF(1) - WF(2)
4200 GH = MC * CP(1) * (T6 - T5) * CYLINDER(1) / EFFICIENCY
4340 ETH = WNET / (3600 / 3413) / .746
4346 EC = MC * CP(1) * TO + (RC - SIGMA(1) - 1) / (WC + WF(1)) / CYLINDER(1))
4347 EE = ((ME - WF(2)) / CYLINDER(2)) / (ME * CP(2) * T7 + (1 - (P6 / P9) * -SIGMA(2))
4350 REM
4500 REM *** -------------------------- OUTPUT OF PERFORMANCE INDICES ***
4510 REM ***
4520 REM ***
4550 PRINT "EFFICIENCY" = ;ETH
4560 PRINT "NET SPECIFIC WORK" = ;WNET / (ME * CYLINDER(2))) [BTU/LBTM]
4570 PRINT "POWER" = ;POWER; [HP]
4580 PRINT "POWER DENSITY" = ;POWER / (VE * CYLINDER(2) * 1728); [HP/CUBIC-INCH]
4590 PRINT "MAJ BRAYTON EFFIC. = ;(1 - 1 / (RC -.2857))
4600 IF TEST$ = "YES" THEN BOSUB 9400
4620 END
5000 REM
5010 REM *** EXPANDER SUBROUTINE ***
5020 REM *** VARIABLE SPEED DRIVE VERSION ***
5030 REM ***
5040 FLOW = MC * CYLINDER(1) / CYLINDER(2)
5050 RPM(2) = RPMMAX
5060 MINRPM = 0
5080 IF (MINRPM = RPMMAX) THEN RETURN
5090 CL2 = FLOW / ((E(2) + RPM(2)) / (T6 + R(2) + 60))
5100 U2(2) = (STROKE(2) + RPM(2) * E(2)) / 360
5110 EMACH(1) = SQR (K(2) * E * R(2) + T6)
5120 ZE1 = (AE1) * U(2) / (CE1 * EMACH(1))
5136 IF ZE1 > .894427191 THEN BOSUB 9360
5140 P2 = P6 + (1.25 * ZE1 - 2)
5150 C2 = C1 + P7 + CLRVOL(2)
5160 V7 = C2 / P7
5170 T7 = T6
5180 T8 = T6 + (V7 / V8) ^ (K(2) - 1)
5196 EMACH(2) = SQR (K(2) * E * R(2) + T6)
5200 ZE2 = AE2 * U(2) / (CE2 * EMACH(2))
5210 IF ZE2 > .894427191 THEN BOSUB 9270
5220 P8 = P9 / (1 + 1.25 * ZE2 - 2)
5230 Y = (U(2) / UMAX) + (P8 / P7)
5240 N(2) = 1 + (K(2) - 1) * Y ^ (1 - LAMBDA(2))
5250 VTEST = VB * (PB / P7) ^ (1 / N(2))
5260 IF ((RPM(2) > RPMMAX) AND (V7 > V8)) THEN PRINT "EXPANDER/COMPRESSOR MISMATCHED": STOP
5270 IF ((VTEST / V7 < = .99) AND (RPM(2) > = .999 * RPMMAX)) THEN PRINT "EXPANDER CAPACITY TOO SMALL; VE NOT LARGE ENOUGH": END
5280 IF VTEST / V7 > 1.005 THEN RPMMAX = RPM(2):RPM(2) = (RPM(2) + MINRPM) / 2: BOSUB 5080
5290 IF VTEST / V7 < .995 THEN MINRPM = RPM(2):RPM(2) = RPM(2) + (RPMMA
1 - RPM(2)) / 2: BOSUB 5080
IF RPM(2) > = .995 * RPMMAX THEN PRINT "COMPRESSOR RPM TOO FAST"
RETURN

REM ***--------------------------------------------***
REM *** EXPANDER SUBROUTINE ***
REM *** VARIABLE VOLUME EXPANDER VERSION ***
REM ***--------------------------------------------***

FLOW = MC * CYLINDER(1) / CYLINDER(2)  

VE = VMAX;V7 = VE  
STROKE(2) = (4 * VE) / (PI * (DIAM(2) / 12) ^ 2) + 12  
C1 = FLOW / ((B2) * RPM(2)) / (T6 + K(2) * 60)  
U2 = (STROKE(2) * RPM(2) * B(2)) / 360  
EMACH(1) = SQRT(K(2) * G * (R(2) * T6))  
IE1 = (AE(1) * U(2)) / (CE(1) * EMACH(1))  

IF (IE1 > .894427191) THEN GOSUB 9360  
P7 = P6 * (1 - 1.25 * IE1 ^ 2)  
C2 = C1 + P7 * CLRVL(2)  
V7 = C2 - P7  
T7 = T6  
VB = VE + CLRVL(2)  
TB = T6 * (V7 / VB) * (K2 - 1)  
EMACH(2) = SQRT(K(2) * G * (R(2) + TB))  
IE2 = (AE(2) * U(2)) / (CE(2) * EMACH(2))  

IF (IE2 > .894427191) THEN GOSUB 9370  
P8 = P6 / ((1 - 1.25 * IE2 ^ 2) + 1)  
Y = (U(2) / UMA1) * (P8 / P7)  

N(2) = 1 + (K2 - 1) * Y ^ (1 - LAMBDA(2))  
VT = VB * (P8 / P7) ^ (1 / N(2))  

IF (VE = VMAX AND VTEST / V7 < 1) THEN PRINT "VAR VOL EXPANDER CAPACITY TOO SMALL AT MINIMUM VE AND GIVEN RPM": END  
IF (VE < 1.01 * VSISMALL AND VTEST / V7 > 1) THEN PRINT "VAR VOL EXPANDER CAPACITY TOO LARGE AT MINIMUM VE AND GIVEN RPM": END  
IF VTEST / V7 < .96 THEN VE = (VE + VMAX) / 2: GOTO 5560  
IF VTEST / V7 > 1.02 THEN VMAX = VE; VE = (VE + VSISMALL) / 2; GOTO 5  

RETURN

REM ***--------------------------------------------***
REM *** SUBROUTINE TO DETERMINE ADEQUACY OF EXPANDER SIZE ***
REM ***--------------------------------------------***

SIZE = (RC ^ - (1 / K(1))) * ((DIAM1) / DIAM(2) ^ 2) * (CYLINDER(1) / CYLINDER(2))  
IF SIZE > 1 THEN PRINT "INCREASE EXPANDER SIZE ];RATIO = ":SIZE  
RETURN

REM ***--------------------------------------------***
REM *** SUBROUTINE TO CALCULATE AIR VISCOSITY AND CONDUCTIVITY ***
REM ***--------------------------------------------***

IF (T > 2500) OR (T < 2500) THEN PRINT "ERROR - TEMPERATURE OUT OF RESONABLE RANGE"  
IF (T = 500) THEN I = 1; N = 1  
IF (T = 500) AND (T < 750) THEN I = 2  
IF (T = 750) AND (T < 1500) THEN I = 3  
IF (T = 1500) THEN N = 4  
IF (T = 500) AND (T < 1900) THEN N = 2  
IF (T = 1900) THEN N = 3  

VISCO = MU(I) + (MU(I + 1) - MU(I)) * (T - TMU(I)) / (TMU(I + 1) - TMU(I))  

IF (T > 672) THEN CONVERT KG/SEC TO LBM/FT-SEC  
KAPPA = KAPPA(N) + (KAPPA(N + 1) - KAPPA(N)) * (T - TKAPPA(N)) / (T - TKAPPA(N))
KAPPA(N + 1) = TKAPPA(N)

9225 KAPPA = KAPPA + .5778 / 3600; REM CONVERT W/M-DEG'C > BTU/SEC-FT

-DEF'

9240 RETURN

9300 REM *** SUBROUTINE TO LIST ERROR MESSAGES ***

9340 PRINT 'COMPRESSOR INLET GAS AT SONIC SPEED: INCREASE PISTON/VALVE'

9345 PRINT 'APERTURE OR MEAN INLET FLOW COEFFICIENT'; RETURN

9350 PRINT 'COMPRESSOR EXIT GAS AT SONIC SPEED: INCREASE PISTON/VALVE'

9355 PRINT 'APERTURE OR MEAN EXIT FLOW COEFFICIENT'; RETURN

9360 PRINT 'EXPANDER INLET GAS AT SONIC SPEED: INCREASE PISTON/VALVE'

9365 PRINT 'APERTURE OR MEAN INLET FLOW COEFFICIENT': RETURN

9370 PRINT 'EXPANDER EXIT GAS AT SONIC SPEED: INCREASE PISTON/VALVE'

9375 PRINT 'APERTURE OR MEAN EXIT FLOW COEFFICIENT': RETURN

9380 PRINT 'CLEARANCE VOLUME TOO LARGE FOR THIS PRESSURE RATIO': RETURN

9400 REM *** SUBROUTINE TO PRINT OUTPUT ***

9430 PRINT 'RPM: COMP/EXP = ';RPM1; RPM2

9440 PRINT 'VOL EFF/ADMISS COEFF= ';EV1; EV2

9450 PRINT 'COMPONENT EFFICIENCY= ';EE1; EE2

9470 PRINT 'WORK-COMPRESS/EXPAND= ';WE1; WE2

9480 REM PRINT 'FRICTION WORK = ';WF1; WF2

9490 PRINT 'HEAT INPUT RATE = ';QH1

9500 PRINT 'MASS LOSS, COMP/EXP = ';MA1; MA2

9510 PRINT 'HEAT LOSS RATIO = ';QL1; QL2

9520 PRINT 'COMP./EXP WORK RATIO= ';WC1; WF1; WE1

9530 BOTO 9855

9600 PRINT 'PO =';PO / 144; TAB(25);*T0 = *;T0

9605 PRINT 'P1 =';P1 / 144; TAB(25);*T1 = *;T1

9610 PRINT 'P2 =';P2 / 144; TAB(25);*T2 = *;T2

9615 PRINT 'P3 =';P3 / 144; TAB(25);*T3 = *;T3

9620 PRINT 'P4 =';P4 / 144; TAB(25);*T4 = *;T4

9625 PRINT 'P5 =';P5 / 144; TAB(25);*T5 = *;T5

9630 PRINT 'P6 =';P6 / 144; TAB(25);*T6 = *;T6

9635 PRINT 'P7 =';P7 / 144; TAB(25);*T7 = *;T7

9640 PRINT 'P8 =';P8 / 144; TAB(25);*T8 = *;T8

9645 PRINT 'P9 =';P9 / 144; TAB(25);*T9 = *;T9

9650 PRINT 'P10 =';P10 / 144; TAB(25);*T10 = *;T10

9655 RETURN