On Modeling Engines

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1 Introduction

Understanding how engines work is vital in a world reliant on mechanical systems. Engines convert fuel into mechanical work, powering vehicles and machinery. My research explores the physics behind their operation, linking theory to practical engineering.

Engine thermodynamics is crucial for optimizing performance, efficiency, and emissions. By understanding the principles of thermodynamics, engineers can design engines that are more powerful, fuel-efficient, and environmentally friendly. This report delves into the fundamental concepts of thermodynamics and fluid dynamics, providing a comprehensive analysis of engine operation.

The report is structured as follows:

- **Basics of Thermodynamics:** Introduction to thermodynamics, conservation of energy, and the First Law of Thermodynamics.
- **Second Law of Thermodynamics:** Concept of entropy, implications for engine efficiency, and examples of irreversible processes.
- **Thermodynamic Cycles:** Analysis of different thermodynamic cycles, including the Otto, Diesel, and Carnot cycles.
- **Heat Transfer:** Mechanisms of heat transfer and their significance in engine design.
- **Gas Laws:** Ideal Gas Law, Van der Waals equation, and real gas considerations.
- **Navier-Stokes Equations:** Fluid dynamics equations and their applications in engine simulations.
- **Engine Specific Processes:** Detailed analysis of the four-stroke cycle and engine-specific processes.
- **Efficiency and Energy Loss:** Factors affecting engine efficiency and methods to quantify energy losses.

- **Scavenging:** Importance of scavenging in engine performance and different scavenging systems.
- **Simulation Workflow:** Step-by-step process for modeling the engine's thermodynamic cycle.
- **Coding the Model:** Implementation of the thermodynamic model and numerical solution.

2 Basics of Thermodynamics

Thermodynamics is the branch of physics that studies the relationships between heat, energy, and work. It provides the foundational principles required to analyse and understand the operation of engines. By examining how energy is conserved and transformed, we can model engine behavior effectively [1, 4].

2.1 Historical Development and Significance

The study of thermodynamics began in the 19th century with the work of scientists like Sadi Carnot, Rudolf Clausius, and William Thomson (Lord Kelvin). Their research laid the groundwork for understanding heat engines and the principles of energy conservation and transformation. Thermodynamics has since become a cornerstone of engineering, enabling the design of efficient engines, power plants, and refrigeration systems.

2.2 Key Concepts: Energy, Heat, and Work

Energy is the capacity to do work or produce heat. It exists in various forms, including kinetic, potential, thermal, and chemical energy. In thermodynamics, we focus on the transfer and transformation of energy within a system.

Heat is a form of energy transfer that occurs due to a temperature difference between a system and its surroundings. It flows from a region of higher temperature to a region of lower temperature.

Work is another form of energy transfer that occurs when a force is applied to move an object over a distance. In engines, work is done by the expanding gases on the piston, converting thermal energy into mechanical energy.

2.3 Conservation of Energy

The principle of conservation of energy is central to thermodynamics. It states that energy cannot be created or destroyed; it can only change forms. This principle forms the basis of the First Law of Thermodynamics, which is applied to both closed and open systems [3].

2.3.1 First Law of Thermodynamics

The First Law of Thermodynamics expresses the principle of energy conservation and is given by:

$$\Delta U = Q - W \tag{1}$$

where ΔU is the change in internal energy of a system, Q is the heat added to the system, and W is the work done by the system [1]. This law governs how fuel's chemical energy is converted into mechanical work and heat in an engine, with the internal energy of the gases changing as heat is transferred and work is performed during different strokes of the cycle [2].

To further understand this equation: - ΔU represents the total internal energy change within the system, including molecular kinetic and potential energies. - Q is the heat transfer into the system, occurring due to a temperature difference between the system and its surroundings. - W denotes the work done by the system, which occurs when a force moves an object over a distance.

This equation states that energy added to the system as heat is either used to increase its internal energy or to perform work on the surroundings. In essence, this formulation of the First Law enforces the conservation of energy, meaning energy can neither be created nor destroyed, only transformed between different forms.

For a closed system (no mass transfer across boundaries), the First Law simplifies to:

$$\Delta U = Q - W \tag{2}$$

However, for an open system (where both mass and energy can cross boundaries), it is expressed as:

$$\dot{Q} - \dot{W} = \frac{d}{dt}\left(\int_V u\, dV\right) + \dot{m}_{in}h_{in} - \dot{m}_{out}h_{out} \tag{3}$$

where:

- $\dot{Q}$ is the rate of heat transfer into the system.
- $\dot{W}$ is the rate of work done by the system.
- u represents internal energy per unit mass within the volume V.
- h denotes specific enthalpy, while $\dot{m}$ represents mass flow rates at inlets and outlets.

In internal combustion engines, these equations describe how energy enters as chemical potential in fuel, is released as heat during combustion, and then exits as mechanical work or waste heat in the exhaust. This understanding is crucial for optimizing engine efficiency and performance [3, 2].

2.4 Entropy and the Second Law of Thermodynamics

Entropy measures a system's disorder and increases in any real process. The Second Law states that no heat engine can be 100% efficient because some entropy generation is inevitable. In engines, irreversible processes like friction and heat loss increase entropy, reducing efficiency.

2.4.1 Second Law of Thermodynamics

The Second Law of Thermodynamics is commonly expressed as:

$$\Delta S \geq 0 \tag{4}$$

where ΔS is the change in entropy of a system. This law states that the total entropy of an isolated system never decreases, and natural processes tend to move towards a state of maximum entropy.

For heat engines, the Second Law implies that it is impossible to convert all the heat energy into work, with some energy always being lost as waste heat. This limitation arises due to the increase in entropy during the conversion of energy.

To understand the Second Law more rigorously, let's consider a reversible heat engine operating between two thermal reservoirs: one at temperature T_H (hot) and the other at temperature T_C (cold). Let the heat transferred from the hot reservoir be Q_H, and the heat rejected to the cold reservoir be Q_C. The efficiency of a reversible heat engine, such as the Carnot engine, is given by:

$$\eta = 1 - \frac{T_C}{T_H} \tag{5}$$

This equation shows the maximum efficiency achievable by a heat engine, which depends on the temperatures of the hot and cold reservoirs.

Next, consider the entropy change associated with the heat transfer to and from the two reservoirs. The change in entropy of a reservoir is defined as:

$$\Delta S = \frac{Q}{T} \tag{6}$$

where Q is the heat transferred, and T is the temperature at which the transfer occurs. For the hot reservoir, the entropy change is:

$$\Delta S_H = -\frac{Q_H}{T_H} \tag{7}$$

Since heat is lost from the hot reservoir, the change in entropy is negative. For the cold reservoir, the entropy change is:

$$\Delta S_C = \frac{Q_C}{T_C} \tag{8}$$

Since heat is added to the cold reservoir, the change in entropy is positive.

For a reversible process, the total entropy change of the system and the surroundings is zero:

$$\Delta S_{\text{total}} = \Delta S_H + \Delta S_C = 0 \tag{9}$$

Substituting the expressions for ΔS_H and ΔS_C, we get:

$$-\frac{Q_H}{T_H} + \frac{Q_C}{T_C} = 0$$

Rearranging this, we find the relation between the heat exchanged in a reversible process:

$$\frac{Q_H}{T_H} = \frac{Q_C}{T_C}$$

This equation shows that for a reversible process, the heat exchanged between the two reservoirs is proportionally related to the temperatures of the reservoirs.

However, for irreversible processes, the total entropy change must be greater than zero. This accounts for the fact that some energy is irreversibly dissipated as waste heat, and the total entropy increases. For a real (irreversible) process, the total entropy change is:

$$\Delta S_{\text{total}} = \Delta S_{\text{system}} + \Delta S_{\text{surroundings}} \geq 0 \tag{10}$$

This inequality confirms that any real process results in an increase in total entropy, ensuring that no process can achieve 100% efficiency. The Second Law of Thermodynamics places a fundamental limit on the efficiency of all energy conversion systems.

Thus, the Second Law is crucial in thermodynamics, governing energy dispersal and ensuring the irreversibility of natural processes. No process can be completely efficient without violating the entropy principle.

2.4.2 Implications for Engine Efficiency

The Second Law has significant implications for engine efficiency. It sets an upper limit on the efficiency of any heat engine, known as the Carnot efficiency:

$$\eta_{\text{Carnot}} = 1 - \frac{T_{\text{cold}}}{T_{\text{hot}}} \tag{11}$$

Where T_{hot} is the temperature of the heat source and T_{cold} is the temperature of the heat sink. This equation shows that the efficiency of a heat engine depends on the temperature difference between the heat source and the heat sink. Higher temperature differences result in higher efficiencies.

2.4.3 Irreversible Processes and Entropy Generation

In real engines, several irreversible processes contribute to entropy generation and reduce efficiency:

- **Friction:** Mechanical friction between moving parts converts useful work into heat, increasing entropy.
- **Heat Loss:** Heat transfer to the surroundings through conduction, convection, and radiation increases entropy.
- **Incomplete Combustion:** Incomplete combustion of fuel results in unburned hydrocarbons and carbon monoxide, increasing entropy.
- **Pumping Losses:** Energy expended in moving gases during intake and exhaust strokes increases entropy.

Understanding and minimizing these irreversible processes is crucial for improving engine efficiency and performance.

2.4.4 T-S Diagram of the Otto Cycle

A temperature-entropy (T-S) diagram helps visualize heat addition and rejection. For the Otto cycle:

- Process 1–2: The piston moves from the bottom dead centre to the top dead centre compressing the fuel-air mixture (charge) in an adiabatic compression.
- Process 2–3: Heat is added to the charge from an external source (this spark plug, as well as the release of energy from the burning of the fuel), at constant volume.
- Process 3–4: The piston expands adiabaticity or isentropically.
- Process 4–1: Heat is rejected at constant volume.

2.4.5 Heat Capacity and the Ratio of Specific Heats

Heat capacity at constant volume (c_v) relates to changes in internal energy, while heat capacity at constant pressure (c_p) also accounts for work done by expansion. The ratio $\gamma = c_p/c_v$ is crucial in modeling adiabatic processes and influences compression/expansion behavior in engines.

2.4.6 Other Thermodynamic Cycles

Otto Cycle: Used in spark-ignition engines.
Diesel Cycle: Differs by heat addition occurring at near-constant pressure.
Carnot Cycle: Theoretically the most efficient, but not practical for engines.
Comparing their efficiencies shows that higher compression ratios and more idealized heat addition can yield greater efficiency, but real engines face losses.

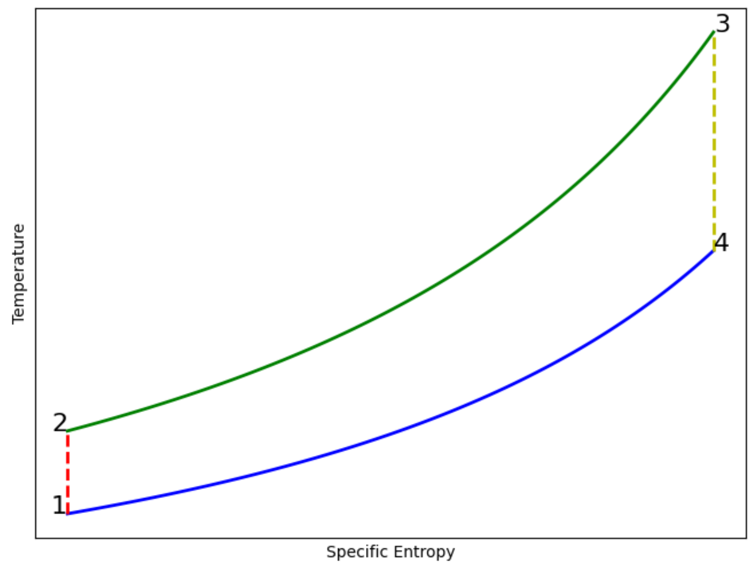

Figure 1: Ideal Otto cycle on a T-S diagram

2.5 Thermodynamic Cycles

Thermodynamic cycles are fundamental to understanding how engines convert heat into work. Each cycle represents a series of processes that return a system to its initial state, allowing for continuous operation. The most common cycles in engine thermodynamics are the Otto, Diesel, and Carnot cycles.

2.5.1 Otto Cycle

The Otto cycle is used in spark-ignition internal combustion engines, such as those found in most gasoline-powered vehicles. It consists of four processes:

- **Adiabatic Compression (1-2):** The air-fuel mixture is compressed, increasing its pressure and temperature without heat transfer.
- **Isochoric Heat Addition (2-3):** Heat is added at constant volume, increasing the pressure and temperature.
- **Adiabatic Expansion (3-4):** The high-pressure gases expand, doing work on the piston and decreasing in pressure and temperature without heat transfer.

- **Isochoric Heat Rejection (4-1):** Heat is rejected at constant volume, returning the system to its initial state.

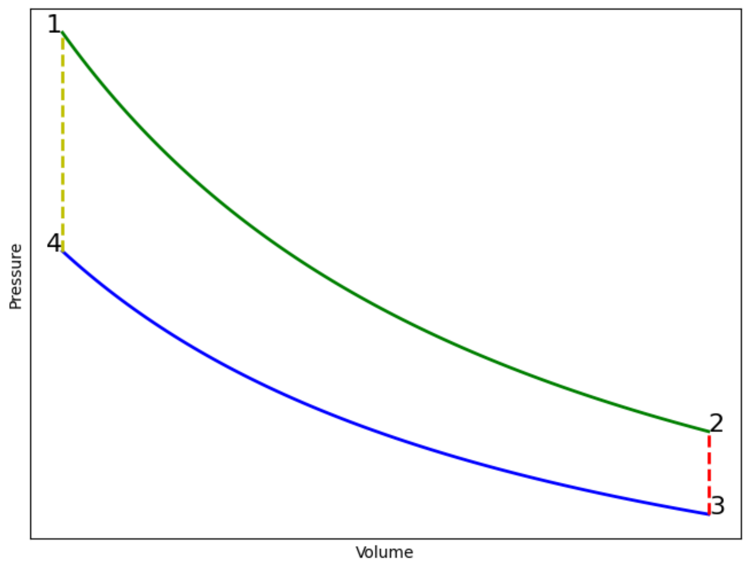

Figure 2: Ideal Otto cycle on a P-V diagram

The efficiency of the Otto cycle is given by:

$$\eta_{\text{Otto}} = 1 - \frac{1}{r^{\gamma-1}} \tag{12}$$

Where:

- r is the compression ratio ($\frac{V_{\text{BDC}}}{V_{\text{TDC}}}$).
- γ is the ratio of specific heats ($\frac{c_p}{c_v}$).

2.5.2 Diesel Cycle

The Diesel cycle is used in compression-ignition engines, such as those found in diesel-powered vehicles. It consists of four processes:

- **Adiabatic Compression (1-2):** The air is compressed, increasing its pressure and temperature without heat transfer.
- **Isobaric Heat Addition (2-3):** Heat is added at constant pressure, increasing the temperature and volume.

- **Adiabatic Expansion (3-4):** The high-pressure gases expand, doing work on the piston and decreasing in pressure and temperature without heat transfer.
- **Isochoric Heat Rejection (4-1):** Heat is rejected at constant volume, returning the system to its initial state.

The efficiency of the Diesel cycle is given by:

$$\eta_{\text{Diesel}} = 1 - \frac{1}{r^{\gamma-1}} \left(\frac{\rho^{\gamma} - 1}{\gamma(\rho - 1)} \right) \tag{13}$$

Where:

- r is the compression ratio.
- γ is the ratio of specific heats.
- ρ is the cutoff ratio ($\frac{V_3}{V_2}$).

2.5.3 Carnot Cycle

The Carnot cycle is a theoretical cycle that represents the maximum possible efficiency for a heat engine. It consists of four processes:

- **Isothermal Expansion (1-2):** The gas expands at constant temperature, doing work on the surroundings while absorbing heat.
- **Adiabatic Expansion (2-3):** The gas continues to expand without heat transfer, decreasing in temperature.
- **Isothermal Compression (3-4):** The gas is compressed at constant temperature, rejecting heat to the surroundings.
- **Adiabatic Compression (4-1):** The gas is compressed without heat transfer, increasing in temperature.

The efficiency of the Carnot cycle is given by:

$$\eta_{\text{Carnot}} = 1 - \frac{T_{\text{cold}}}{T_{\text{hot}}} \tag{14}$$

Where:

- T_{hot} is the temperature of the heat source.
- T_{cold} is the temperature of the heat sink.

2.5.4 Comparison of Cycles

The Carnot cycle represents the upper limit of efficiency, but it is not practical for real engines due to its idealized assumptions. The Otto and Diesel cycles are more representative of actual engine operation. The Diesel cycle typically has higher efficiency than the Otto cycle due to higher compression ratios and more efficient heat addition. However, Diesel engines are generally heavier and more expensive to manufacture.

2.6 Heat Transfer

Heat transfer is a critical aspect of engine design, as it affects performance, efficiency, and durability. There are three primary modes of heat transfer: conduction, convection, and radiation.

2.6.1 Conduction

Conduction is the transfer of heat through a solid material due to a temperature gradient. It is governed by Fourier's Law:

$$Q = -kA\frac{dT}{dx} \tag{15}$$

Where:

- Q is the heat transfer rate.
- k is the thermal conductivity of the material.
- A is the cross-sectional area through which heat is conducted.
- $\frac{dT}{dx}$ is the temperature gradient.

This equation can be seen as common sense, as shows that heat transfer rate is proportional to Area for a given temperature gradient, and also that a larger temperature gradient causes a faster ate of heat transfer.

In engines, conduction occurs through components like cylinder walls, pistons, and cylinder heads.

2.6.2 Convection

Convection is the transfer of heat between a solid surface and a fluid (liquid or gas) in motion. It is described by Newton's Law of Cooling:

$$Q = hA(T_s - T_\infty) \tag{16}$$

Where:

- Q is the heat transfer rate.
- h is the convective heat transfer coefficient.

- A is the surface area.
- T_s is the surface temperature.
- T_∞ is the fluid temperature far from the surface.

Convection is important in engine cooling systems, where heat is transferred from engine components to the coolant or air.

Newton's Law of Cooling is an empirical relationship that describes convective heat transfer at a boundary. It can be derived using fundamental principles of heat transfer.

Step 1: Fourier's Law and Energy Balance

At a solid-fluid interface, heat is transferred via both conduction and convection. Consider a thin layer of fluid adjacent to the solid surface. Under steady-state conditions, the heat conducted through this layer must equal the heat convected away.

- According to Fourier's Law of Heat Conduction, the heat flux q'' at the surface is:
$$q'' = -k \frac{dT}{dy}\bigg|_{y=0} \tag{17}$$
where k is the thermal conductivity of the fluid, and dT/dy is the temperature gradient in the normal direction at the surface.
- The energy balance at the interface requires that the same amount of heat is convected into the bulk fluid. Convection is driven by the temperature difference between the surface temperature T_s and the bulk fluid temperature T_∞.

Step 2: Defining the Convective Heat Transfer Coefficient

Experimental observations suggest that the heat transfer rate per unit area due to convection is proportional to this temperature difference:

$$q'' = h(T_s - T_\infty) \tag{18}$$

where h is the convective heat transfer coefficient, which depends on fluid properties, flow characteristics, and the nature of the boundary layer.

Step 3: Generalizing for Total Heat Transfer Rate

Since the heat flux is defined as $q'' = Q/A$, where Q is the total heat transfer rate and A is the heat transfer surface area, we obtain:

$$\frac{Q}{A} = h(T_s - T_\infty) \tag{19}$$

Multiplying both sides by A, we arrive at Newton's Law of Cooling:

$$Q = hA(T_s - T_\infty) \tag{20}$$

2.6.3 Radiation

Radiation is the transfer of heat through electromagnetic waves. It is governed by the Stefan-Boltzmann Law:

$$Q = \epsilon \sigma A (T_s^4 - T_\infty^4) \tag{21}$$

Where:

- Q is the heat transfer rate.
- ϵ is the emissivity of the surface.
- σ is the Stefan-Boltzmann constant ($5.67 \times 10^{-8}\,\mathrm{W/m^2K^4}$).
- A is the surface area.
- T_s is the surface temperature.
- T_∞ is the temperature of the surroundings.

Radiation is significant in high-temperature engine components, such as exhaust manifolds and turbochargers.

2.6.4 A rabbit-hole of derivations you needn't read if you're not Zac Baker

It can be derived as follows.

Step 1: Blackbody Radiation and the Stefan-Boltzmann Law

A perfect blackbody is an idealized surface that absorbs and emits all incident radiation. The total energy emitted per unit area by a blackbody is given by the Stefan-Boltzmann equation:

$$E_b = \sigma T^4 \tag{22}$$

where E_b is the emissive power, T is the absolute temperature of the surface, and σ is the Stefan-Boltzmann constant, given by:

$$\sigma = 5.67 \times 10^{-8}\,\mathrm{W/m^2K^4}.$$

Step 2: Introducing Emissivity

Real surfaces do not behave as perfect blackbodies; instead, they emit only a fraction of the radiation. This fraction is quantified by the **emissivity** ϵ, which ranges from 0 (perfect reflector) to 1 (perfect blackbody). The radiation emitted by a real surface is:

$$E = \epsilon \sigma T^4. \tag{23}$$

Step 3: Net Radiative Heat Exchange

For radiative heat transfer between a surface at temperature T_s and its surroundings at temperature T_∞, the net radiative heat loss from the surface is given by:

$$Q = \epsilon \sigma A (T_s^4 - T_\infty^4), \tag{24}$$

where A is the surface area.

Derivation of the Stefan-Boltzmann Law

The Stefan-Boltzmann Law states that the total radiative energy emitted per unit area of a blackbody is proportional to the fourth power of its absolute temperature:

$$E_b = \sigma T^4. \tag{25}$$

This law can be derived by integrating Planck's Law over all wavelengths.

Step 1: Planck's Law for Blackbody Radiation

Planck's Law describes the spectral radiance $I_\lambda(T)$, which gives the energy emitted per unit area, per unit solid angle, per unit wavelength:

$$I_\lambda(T) = \frac{2\pi hc^2}{\lambda^5} \frac{1}{e^{\frac{hc}{\lambda k_B T}} - 1}. \tag{26}$$

Step 2: Total Emissive Power from a Blackbody

The total power radiated per unit area across all wavelengths is given by integrating the spectral radiance over all wavelengths and over a hemisphere (solid angle 2π):

$$E_b = \pi \int_0^\infty I_\lambda(T)\, d\lambda. \tag{27}$$

Substituting Planck's Law:

$$E_b = \pi \int_0^\infty \frac{2\pi hc^2}{\lambda^5} \frac{1}{e^{\frac{hc}{\lambda k_B T}} - 1} d\lambda. \tag{28}$$

Step 3: Changing Variables for Integration

Define a new dimensionless variable:

$$x = \frac{hc}{\lambda k_B T}, \quad \text{so that} \quad dx = -\frac{hc}{k_B T} \frac{d\lambda}{\lambda^2}. \tag{29}$$

Rewriting the differential:

$$d\lambda = -\frac{k_B T}{hc} \lambda^2 dx. \tag{30}$$

Since $\lambda = \frac{hc}{k_B T} \frac{1}{x}$, substituting these into the integral:

$$E_b = \pi \int_0^\infty \frac{2\pi hc^2}{\lambda^5} \frac{1}{e^{\frac{hc}{\lambda k_B T}} - 1} \left(-\frac{k_B T}{hc} \lambda^2 dx \right). \tag{31}$$

Simplifying:

$$E_b = 2\pi^5 \frac{k_B^4}{h^3 c^2} T^4 \int_0^\infty \frac{x^3}{e^x - 1} dx. \tag{32}$$

The remaining integral:

$$\int_0^\infty \frac{x^3}{e^x - 1} dx = \frac{\pi^4}{15} \tag{33}$$

is a standard result from Bose-Einstein integrals. Substituting this:

$$E_b = \frac{2\pi^5 k_B^4}{15 h^3 c^2} T^4. \tag{34}$$

Step 4: Defining the Stefan-Boltzmann Constant

The Stefan-Boltzmann constant is defined as:

$$\sigma = \frac{2\pi^5 k_B^4}{15 h^3 c^2} = 5.67 \times 10^{-8}\,\mathrm{W/m^2K^4}. \tag{35}$$

Thus, the Stefan-Boltzmann Law is obtained:

$$E_b = \sigma T^4. \tag{36}$$

Derivation of Planck's Law

Planck's Law describes the spectral radiance of a blackbody, which is the power emitted per unit area, per unit solid angle, per unit wavelength. It is given by:

$$I_\lambda(T) = \frac{2\pi hc^2}{\lambda^5} \frac{1}{e^{\frac{hc}{\lambda k_B T}} - 1}. \tag{37}$$

This law can be derived using quantum mechanics and statistical physics.

Step 1: Modeling Radiation as a Collection of Oscillators

A blackbody cavity can be modeled as an enclosure filled with electromagnetic radiation in thermal equilibrium with its walls. The standing electromagnetic waves inside the cavity behave as quantized harmonic oscillators.

Each mode of electromagnetic radiation in a cavity corresponds to a standing wave with frequency ν, and its energy is given by:

$$E_n = nh\nu, \quad n = 0, 1, 2, \ldots \tag{38}$$

where:

- h is Planck's constant (6.626×10^{-34} J·s),
- ν is the frequency of the wave,
- n is the quantum number representing discrete energy levels.

Step 2: Bose-Einstein Statistics for Photons

Since photons are bosons, they follow Bose-Einstein statistics. The mean number of photons in a given mode at thermal equilibrium is given by the Bose-Einstein distribution:

$$\langle n \rangle = \frac{1}{e^{\frac{h\nu}{k_B T}} - 1}. \tag{39}$$

Step 3: Energy Density of Radiation in the Cavity

The energy density $u(\nu)d\nu$ (energy per unit volume per unit frequency) can be found by multiplying the average energy per mode by the density of available states in the cavity.

- The total energy in a single mode is given by:

$$E_{\text{mode}} = \langle n \rangle h\nu = \frac{h\nu}{e^{\frac{h\nu}{k_B T}} - 1}. \tag{40}$$

- The number of electromagnetic modes per unit volume in the frequency range $d\nu$ is:

$$g(\nu)d\nu = \frac{8\pi\nu^2}{c^3}d\nu. \tag{41}$$

Thus, the energy density of radiation inside the cavity is given by:

$$u(\nu)d\nu = \frac{8\pi h\nu^3}{c^3}\frac{1}{e^{\frac{h\nu}{k_B T}} - 1}d\nu. \tag{42}$$

Step 4: Converting to Spectral Radiance

The spectral radiance I_ν, which is the power emitted per unit area per unit solid angle per unit frequency, is related to the energy density by:

$$I_\nu = \frac{c}{4}u(\nu). \tag{43}$$

Substituting for $u(\nu)$:

$$I_\nu(T) = \frac{2h\nu^3}{c^2}\frac{1}{e^{\frac{h\nu}{k_B T}} - 1}. \tag{44}$$

Step 5: Converting to Wavelength Form

Since frequency and wavelength are related by $\nu = c/\lambda$, we transform the equation in terms of λ:

$$I_\lambda(T) = I_\nu \left| \frac{d\nu}{d\lambda} \right| = \frac{2\pi hc^2}{\lambda^5} \frac{1}{e^{\frac{hc}{\lambda k_B T}} - 1}. \tag{45}$$

$$\langle n \rangle = \frac{1}{e^{\frac{E-\mu}{k_B T}} - 1}. \tag{46}$$

Bose-Einstein distribution

This can be derived using the principles of quantum statistical mechanics.

Step 1: Bose-Einstein Statistics and Quantum States

Consider a system of indistinguishable bosons, each occupying discrete energy states E_i. Unlike fermions, bosons do not obey the Pauli exclusion principle, meaning multiple bosons can occupy the same state.

The system is described by a grand canonical ensemble, where the total number of particles can fluctuate, and the probability of a state depends on the chemical potential μ, which enforces conservation of particle number.

Step 2: Partition Function for a Single Quantum State

For a given quantum state with energy E, the number of bosons in that state can be $n = 0, 1, 2, \ldots$. The probability of finding exactly n bosons in this state follows the Boltzmann factor:

$$P_n = \frac{e^{-\beta(E-\mu)n}}{Z}, \tag{47}$$

where:

- $\beta = \frac{1}{k_B T}$ (inverse temperature),
- μ is the chemical potential,
- Z is the partition function ensuring proper normalization.

Step 3: Partition Function for a Single State

The partition function sums over all possible occupations:

$$Z = \sum_{n=0}^{\infty} e^{-\beta(E-\mu)n}. \tag{48}$$

This is an infinite geometric series of the form:

$$\sum_{n=0}^{\infty} r^n = \frac{1}{1-r}, \quad \text{for } |r| < 1. \tag{49}$$

Here, $r = e^{-\beta(E-\mu)}$, so the partition function becomes:

$$Z = \frac{1}{1 - e^{-\beta(E-\mu)}}. \tag{50}$$

Step 4: Computing the Expected Occupation Number

The average number of particles in this state is given by:

$$\langle n \rangle = \sum_{n=0}^{\infty} n P_n. \tag{51}$$

Using the definition of P_n:

$$\langle n \rangle = \frac{1}{Z} \sum_{n=0}^{\infty} n e^{-\beta(E-\mu)n}. \tag{52}$$

The sum in the numerator is:

$$\sum_{n=0}^{\infty} n r^n = \frac{r}{(1-r)^2}, \quad \text{for } |r| < 1. \tag{53}$$

Substituting $r = e^{-\beta(E-\mu)}$:

$$\sum_{n=0}^{\infty} n e^{-\beta(E-\mu)n} = \frac{e^{-\beta(E-\mu)}}{(1 - e^{-\beta(E-\mu)})^2}. \tag{54}$$

Dividing by Z, we obtain the Bose-Einstein distribution:

$$\langle n \rangle = \frac{1}{e^{\beta(E-\mu)} - 1}. \tag{55}$$

Step 5: Application to Photons

For photons, the chemical potential is zero ($\mu = 0$), because photons can be freely created or destroyed in thermal equilibrium. This simplifies the Bose-Einstein distribution to:

$$\langle n \rangle = \frac{1}{e^{h\nu/k_B T} - 1}. \tag{56}$$

2.6.5 Importance of Heat Transfer in Engine Design

Effective heat transfer management is crucial for engine performance and longevity. Excessive heat can lead to component failure, reduced efficiency, and increased emissions. Engine designers use materials with high thermal conductivity, optimise cooling systems, and employ heat shields to manage heat transfer effectively.

2.7 Gas Laws

Understanding the behavior of gases under various conditions of pressure, temperature, and volume is fundamental to the thermodynamic processes occurring within an engine. Gas laws provide the necessary framework for modeling these behaviors, allowing engineers to analyze and predict engine performance accurately.

One of the most important gas laws in this context is the *Ideal Gas Law*, which provides a simplified model for the behavior of gases in an engine. The Ideal Gas Law is expressed as:

$$PV = nRT \tag{57}$$

where P represents the pressure of the gas, V is the volume, n is the number of moles of gas, R is the universal gas constant ($8.314\,\mathrm{J/mol\cdot K}$), and T is the absolute temperature of the gas in Kelvin.

This equation can be derived from a combination of empirical observations and kinetic theory. The kinetic theory of gases postulates that gas pressure results from the constant collisions of gas molecules with the walls of their container. By considering the average kinetic energy of the molecules and how it relates to temperature, we can derive the relationship between pressure, volume, and temperature for an ideal gas. The Ideal Gas Law assumes that gas particles move independently with negligible intermolecular forces and occupy no volume themselves, establishing a direct relationship between the pressure, volume, and temperature of a gas.

In engines, the Ideal Gas Law serves as a useful approximation during the intake and compression strokes, where the behavior of the air-fuel mixture can be approximated as an ideal gas [3]. It allows for estimating cylinder pressures during compression and expansion, modeling the behavior of air-fuel mixtures, and simplifying thermodynamic cycle analysis. By applying the Ideal Gas Law, engineers can predict how changes in temperature or volume will affect the pressure within the cylinder, which is crucial for designing engines that operate efficiently.

However, it is important to recognize that the Ideal Gas Law is a simplification, and real gases often deviate from ideal behavior, especially under conditions of high pressure and temperature typical in internal combustion engines. Under such extreme conditions, intermolecular forces and the finite size of gas molecules become significant, and the assumptions of the Ideal Gas Law no longer hold true. To account for these real gas effects, advanced models such as the *Van der Waals equation* are employed.

The Van der Waals equation introduces correction factors to the Ideal Gas Law to account for the volume occupied by gas molecules and the intermolecular forces between them. It is expressed as:

$$\left(P + \frac{n^2 a}{V^2}\right)(V - nb) = nRT \tag{58}$$

This equation is derived by modifying the Ideal Gas Law to incorporate two key adjustments:

1. Correction for intermolecular forces: The term $\frac{n^2 a}{V^2}$ accounts for the attractive forces between gas molecules. These forces reduce the pressure exerted by the gas, which is reflected by the addition of the $\frac{n^2 a}{V^2}$ term to the pressure.

2. Correction for molecular volume: The term nb accounts for the finite volume of the gas molecules themselves. In the Ideal Gas Law, the volume of the gas molecules is assumed to be negligible, but in reality, they occupy a small but non-zero volume, reducing the available volume for the gas particles to move.

In this equation, a and b are substance-specific constants representing the strength of intermolecular attractions and the volume occupied by the gas molecules, respectively. By incorporating these constants, the Van der Waals equation provides a more accurate representation of gas behavior under conditions where deviations from ideality are significant.

Understanding the differences between the Ideal Gas Law and the Van der Waals equation is crucial for accurate thermodynamic analysis in engines. While the Ideal Gas Law simplifies calculations and is sufficient for many purposes, the Van der Waals equation offers greater precision in modeling gas behavior under high pressures and temperatures. This precision is important for predicting engine performance, optimizing efficiency, and ensuring that engines operate safely under all conditions.

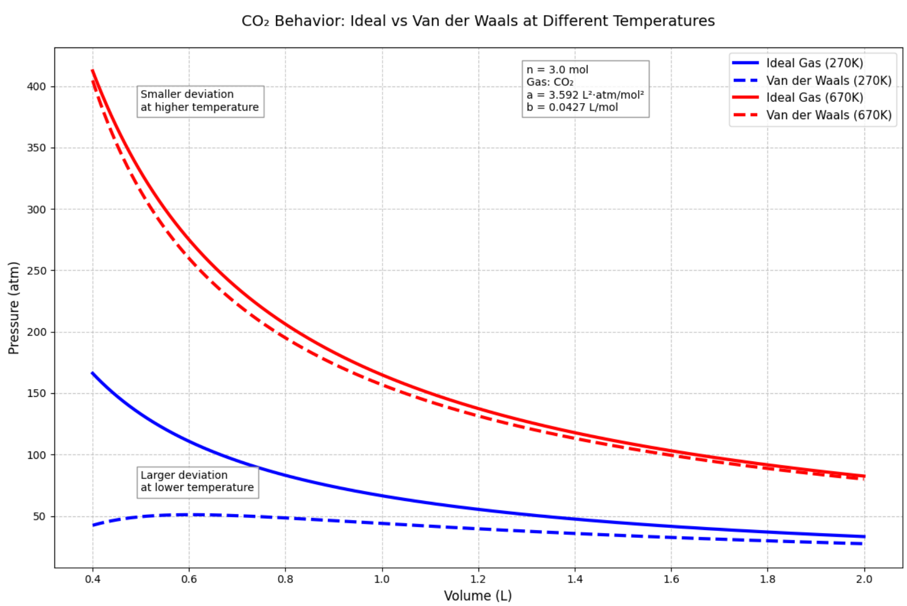

Figure 3: Comparison between Ideal Gas Law and Van der Waals equation predictions under varying pressures and temperatures

2.7.1 Kinetic Theory of Gases & Real Gas Considerations

Kinetic theory assumes random motion of point-like particles with no intermolecular forces, deriving the Ideal Gas Law. Under high pressure and temperature, real gases deviate from ideality. Van der Waals constants a (intermolecular forces) and b (molecular volume) correct for these effects. Other equations (e.g., Redlich-Kwong) improve accuracy under extreme conditions.

For an adiabatic process, there is no heat transfer ($Q = 0$). The First Law of Thermodynamics simplifies to:

$$\Delta U = -W \tag{59}$$

For an ideal gas undergoing an adiabatic process, the relationship between pressure and volume is given by:

$$PV^{\gamma} = \text{constant} \tag{60}$$

Where $\gamma = \frac{c_p}{c_v}$ is the ratio of specific heats. This can be derived from the differential form of the First Law and the definition of specific heats.

2.7.2 Heat Loss

Heat loss is a critical factor in engine thermodynamics, as it affects both efficiency and performance. During engine operation, a significant portion of the energy released during combustion is lost as heat to the surroundings. This heat loss occurs through:

- **Conduction:** Heat transfer through the engine walls and cylinder materials.
- **Convection:** Heat transfer to the surrounding air or cooling system.
- **Radiation:** Emission of thermal energy as electromagnetic waves.

The extent of heat loss depends on factors such as the thermal conductivity of engine materials, the temperature gradient between the engine and surroundings, and the efficiency of the cooling system. Minimizing heat loss is vital for improving the overall thermal efficiency of an engine [2].

Mathematically, heat loss Q_{loss} can be expressed using Fourier's Law for conduction or Newton's Law of Cooling for convection. For conduction, Fourier's Law states that the rate of heat transfer is proportional to the temperature gradient and the thermal conductivity of the material. Specifically, the equation is:

$$Q_{\text{loss}} = -kA\frac{dT}{dx} \tag{61}$$

where k is the thermal conductivity, A is the surface area, and $\frac{dT}{dx}$ is the temperature gradient along the material. This relationship arises because heat flows from high to low and the rate of flow depends on how easily the material conducts heat and how steep the temperature difference is.

Understanding and mitigating heat loss enables engineers to design more efficient engines by optimizing materials and cooling strategies [**?**].

2.8 Navier-Stokes Equations

Fluid dynamics is the study of fluids (liquids and gases) in motion. It is essential for understanding the behavior of gases within an engine, including air intake, fuel-air mixing, combustion, and exhaust processes. The Navier-Stokes equations are fundamental to fluid dynamics, describing the motion of fluid substances by accounting for velocity, pressure, density, and external forces.

The Navier-Stokes equations are derived from Newton's second law applied to a fluid element. They consist of three main equations: conservation of mass, conservation of momentum, and conservation of energy.

Conservation of Mass (Continuity Equation) The continuity equation ensures mass conservation in a fluid flow:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0 \tag{62}$$

Where:

- ρ: Fluid density.
- $\mathbf{u}$: Velocity vector.
- t: Time.

This equation states that the rate of change of mass within a control volume plus the net mass flux across the control volume boundaries is zero.

Conservation of Momentum The conservation of momentum for a fluid element is expressed as:

$$\rho \left(\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla)\mathbf{u} \right) = -\nabla P + \mu \nabla^2 \mathbf{u} + \mathbf{f} \tag{63}$$

Where:

- P: Pressure.
- μ: Dynamic viscosity.
- $\mathbf{f}$: External body forces per unit mass (e.g., gravity).

This equation represents the balance of forces acting on a fluid element, including pressure gradients, viscous forces, and external body forces.

Conservation of Energy The conservation of energy for a fluid element is given by:

$$\rho \left(\frac{\partial e}{\partial t} + (\mathbf{u} \cdot \nabla) e \right) = -\nabla \cdot \mathbf{q} + \Phi + \mathbf{f} \cdot \mathbf{u} \tag{64}$$

Where:

- e: Internal energy per unit mass.
- $\mathbf{q}$: Heat flux vector.
- Φ: Dissipation function representing viscous dissipation.

This equation accounts for the rate of change of internal energy, heat conduction, viscous dissipation, and work done by external forces.

2.8.1 Applications in Engine Simulations

The Navier-Stokes equations are essential for modeling complex fluid dynamics in engines, including:

- **Intake and Exhaust Flows:** Simulating air and exhaust gas flow through intake and exhaust manifolds, valves, and ports.
- **Combustion Processes:** Modeling fuel-air mixing, flame propagation, and heat release in the combustion chamber.
- **Turbulence:** Capturing turbulent flow structures that enhance mixing and combustion efficiency.
- **Heat Transfer:** Analyzing heat transfer between gases and engine components, such as cylinder walls and pistons.

2.8.2 Turbulence Modeling

Turbulence is a key aspect of fluid flow in engines, characterized by chaotic and irregular motion. Direct Numerical Simulation (DNS) of turbulence is computationally expensive, so engineers use turbulence models such as:

- **Reynolds-Averaged Navier-Stokes (RANS):** Simplifies turbulence by averaging the equations and introducing turbulence models like k-epsilon and k-omega.
- **Large Eddy Simulation (LES):** Resolves large turbulent structures while modeling smaller scales.
- **Detached Eddy Simulation (DES):** Combines RANS and LES for efficient simulation of both near-wall and free-stream turbulence.

2.8.3 Numerical Methods for Solving Navier-Stokes Equations

Solving the Navier-Stokes equations requires numerical methods, including:

- **Finite Difference Method (FDM):** Approximates derivatives using differences between grid points.
- **Finite Volume Method (FVM):** Conserves fluxes across control volumes, suitable for complex geometries.
- **Finite Element Method (FEM):** Uses variational principles to solve fluid flow problems, offering flexibility in handling complex boundaries.

2.8.4 Boundary Conditions

Proper boundary conditions are crucial for accurate simulations:

- **Inlet and Outlet Boundaries:** Specify velocity, pressure, or mass flow rates.
- **Wall Boundaries:** Apply no-slip conditions for velocity and appropriate thermal conditions for heat transfer.
- **Symmetry Boundaries:** Reduce computational effort by exploiting flow symmetry.

bsectionChallenges and Limitations Despite their power, Navier-Stokes simulations face challenges:

- **Computational Cost:** High-resolution simulations require significant computational resources.
- **Complex Geometries:** Handling intricate engine geometries demands advanced meshing techniques.
- **Turbulence Modeling:** Accurate turbulence models are essential but can be complex to implement.
- **Convergence and Stability:** Ensuring numerical stability and convergence is critical for reliable results.

2.8.5 Importance of Numerical Methods

Numerical methods are crucial for solving the Navier-Stokes equations in practical applications. They enable engineers to simulate complex fluid dynamics in engines, including intake and exhaust flows, combustion processes, and heat transfer. Computational Fluid Dynamics (CFD) techniques provide detailed insights into gas flow behavior, helping optimize engine performance and efficiency.

3 Engine Specific Processes

This section focuses on the engine-specific processes that occur during the operation of a four-stroke internal combustion engine. The cycle comprises four distinct strokes: intake, compression, power, and exhaust. Each stroke involves unique thermodynamic processes that can be modeled using fundamental equations.

3.0.1 Intake Stroke

The intake stroke begins when the intake valve opens, allowing a mixture of air and fuel (or just air in diesel engines) to enter the cylinder as the piston moves downward. This stroke can be approximated as an isobaric process, where the pressure remains nearly constant.

The mass of air-fuel mixture entering the cylinder can be modeled using the Ideal Gas Law, which as seen before is:

$$PV = nRT \tag{65}$$

Key considerations during this stroke include volumetric efficiency, which accounts for how effectively the cylinder is filled with the air-fuel mixture [2].

3.0.2 Compression Stroke

In the compression stroke, the piston moves upward, compressing the air-fuel mixture. This process can be modeled as adiabatic (no heat transfer), assuming ideal insulation of the cylinder.

The relationship between pressure and volume during adiabatic compression is given by:

$$PV^\gamma = \text{constant} \tag{66}$$

The compression ratio r is defined as:

$$r = \frac{V_{\text{BDC}}}{V_{\text{TDC}}} \tag{67}$$

Where V_{BDC} is the volume at bottom dead center and V_{TDC} is the volume at top dead center.

The final pressure and temperature at the end of compression can be calculated as:

$$P_2 = P_1 r^\gamma \quad \text{and} \quad T_2 = T_1 r^{\gamma-1} \tag{68}$$

3.0.3 Power Stroke

The power stroke begins with combustion, rapidly increasing pressure and temperature within the cylinder. This process can be approximated as constant-volume heat addition (isochoric process), followed by an adiabatic expansion as the piston moves downward.

During the isochoric heat addition, the increase in pressure is calculated as:

$$P_3 = P_2 + \frac{Q_{\text{in}}}{V_{\text{TDC}}} \tag{69}$$

Where Q_{in} is the heat energy released during combustion.

The adiabatic expansion is governed by the same relationship as the compression stroke:

$$PV^{\gamma} = \text{constant} \tag{70}$$

The work output during this stroke is given by:

$$W_{\text{power}} = \int_{V_{\text{TDC}}}^{V_{\text{BDC}}} P\,dV \tag{71}$$

3.0.4 Exhaust Stroke

In the exhaust stroke, the piston moves upward, expelling burned gases through the exhaust valve. This stroke is modeled as an isobaric process, where pressure remains nearly constant at exhaust manifold pressure P_{exhaust}.

The work required to expel the gases is given by:

$$W_{\text{exhaust}} = P_{\text{exhaust}}(V_{\text{BDC}} - V_{\text{TDC}}) \tag{72}$$

Key considerations include backpressure in the exhaust manifold reducing engine efficiency [3].

Together, these strokes form the basis of the thermodynamic cycle of an internal combustion engine, with each stroke contributing to the overall energy transformation process.

3.0.5 Intake and Exhaust Valve Timing

Valve timing affects performance and volumetric efficiency. *Valve overlap* can improve scavenging but risk backflow. Designers optimize timing for high power and fuel economy.

3.0.6 Volumetric Efficiency

Defines how effectively air fills the cylinder. Factors include manifold design, valve events, and flow losses. Higher volumetric efficiency improves power output.

3.0.7 Combustion Process

Combustion releases chemical energy as heat. In spark-ignition engines, a flame front propagates through the mixture. Complete combustion requires correct air-fuel ratio, ignition timing, and proper turbulence.

3.0.8 Indicated, Brake, and Friction Work

Indicated work is the total work from in-cylinder pressures. **Brake work** is the useful work at the crankshaft. **Friction work** is lost to friction in moving parts. Engine efficiency depends on minimizing friction and other losses.

4 Efficiency & Energy Loss

Efficiency is a critical parameter in engine design, representing how effectively the chemical energy of fuel is converted into useful mechanical work. For internal combustion engines, the thermal efficiency is defined as:

$$\eta_{\text{thermal}} = \frac{W_{\text{net}}}{Q_{\text{in}}} \tag{73}$$

Where:

- W_{net}: Net work output.
- Q_{in}: Heat energy supplied during combustion.

The maximum theoretical efficiency for an idealized engine operating on the Otto cycle is given by:

$$\eta_{\text{otto}} = 1 - \frac{1}{r^{\gamma-1}} \tag{74}$$

Where:

- r: Compression ratio.
- γ: Ratio of specific heats (c_p/c_v).

4.0.1 Energy Loss

In practical engines, several factors reduce efficiency:

- **Heat Loss:** Significant energy is lost to the surroundings through conduction, convection, and radiation.
- **Friction Losses:** Mechanical friction between moving parts consumes part of the energy.
- **Incomplete Combustion:** Some fuel remains unburned or partially burned, reducing energy conversion.
- **Pumping Losses:** Energy is expended in moving gases during intake and exhaust strokes.

Quantifying these losses helps identify opportunities for improving engine design and efficiency [2, 1].

4.1 Scavenging

Scavenging refers to the process of expelling exhaust gases from the cylinder and replacing them with a fresh air-fuel mixture. Efficient scavenging ensures complete removal of exhaust gases while minimizing energy losses and backflow.

Types of Scavenging:

- **Cross-flow scavenging:** Fresh air enters from one side while exhaust exits from the opposite side.
- **Loop scavenging:** Fresh air follows a loop path to push out exhaust gases.
- **Uniflow scavenging:** Both intake and exhaust occur in the same direction, providing high efficiency.

Scavenging efficiency can be expressed as:

$$\eta_{\text{scavenging}} = \frac{\text{Mass of fresh air}}{\text{Mass of cylinder contents}} \tag{75}$$

Effective scavenging improves combustion, reduces residual gases, and enhances overall engine performance. It requires precise timing of intake and exhaust valve operation to avoid overlapping flows [2].

4.1.1 Scavenging Systems

Cross-flow, loop, uniflow scavenging each offer different advantages (packaging, flow efficiency, complexity). Proper scavenging reduces residual gases, enhancing performance.

4.2 More Gases

The behavior of gases within an engine becomes increasingly complex when accounting for real gas effects, turbulence, and compressibility.

4.2.1 Navier-Stokes in Engine Simulations

The Navier-Stokes equations are essential for modeling complex fluid dynamics in engines, including:

- **Intake and Exhaust Flows:** Simulating air and exhaust gas flow through intake and exhaust manifolds, valves, and ports.
- **Combustion Processes:** Modeling fuel-air mixing, flame propagation, and heat release in the combustion chamber.
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4.2.2 Turbulence Modeling

Turbulence is a key aspect of fluid flow in engines, characterized by chaotic and irregular motion. Direct Numerical Simulation (DNS) of turbulence is computationally expensive, so engineers use turbulence models such as:

- **Reynolds-Averaged Navier-Stokes (RANS):** Simplifies turbulence by averaging the equations and introducing turbulence models like k-epsilon and k-omega.
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4.2.3 Numerical Methods for Solving Navier-Stokes Equations

Solving the Navier-Stokes equations requires numerical methods, including:

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Proper boundary conditions are crucial for accurate simulations:

- **Inlet and Outlet Boundaries:** Specify velocity, pressure, or mass flow rates.
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- **Symmetry Boundaries:** Reduce computational effort by exploiting flow symmetry.

4.2.5 Challenges and Limitations

Despite their power, Navier-Stokes simulations face challenges:

- **Computational Cost:** High-resolution simulations require significant computational resources.
- **Complex Geometries:** Handling intricate engine geometries demands advanced meshing techniques.

- **Turbulence Modeling:** Accurate turbulence models are essential but can be complex to implement.
- **Convergence and Stability:** Ensuring numerical stability and convergence is critical for reliable results.

4.2.6 Future Directions

Advancements in computational power and algorithms continue to enhance Navier-Stokes simulations:

- **High-Performance Computing (HPC):** Leveraging HPC resources for large-scale simulations.
- **Machine Learning:** Integrating machine learning techniques to improve turbulence modeling and reduce computational cost.
- **Multiphysics Simulations:** Coupling fluid dynamics with other physical phenomena, such as chemical reactions and structural mechanics.

5 Simulation Workflow

The simulation workflow outlines the step-by-step process for modeling the engine's thermodynamic cycle. This involves defining input parameters, implementing mathematical models, and analyzing the results to validate performance.

5.1 1. Define Input Parameters

The first step in the simulation process is defining the key input parameters for the engine model. These include:

- **Engine geometry:** Cylinder bore, stroke, compression ratio, and number of cylinders.
- **Operating conditions:** Intake pressure, temperature, and engine speed (RPM).
- **Fuel properties:** Heat of combustion, air-fuel ratio, and specific heat ratios.
- **Initial conditions:** Pressure, volume, and temperature at the start of the cycle.

5.2 2. Thermodynamic Modeling

Using the input parameters, the thermodynamic processes of the engine are modeled for each stroke.

- **Intake stroke:** Use the Ideal Gas Law to model the mass of the air-fuel mixture entering the cylinder.
- **Compression stroke:** Apply adiabatic compression equations to determine pressure and temperature changes.
- **Power stroke:** Model heat addition using constant-volume assumptions and compute work output using pressure-volume relationships.
- **Exhaust stroke:** Simulate the expulsion of exhaust gases under near-constant pressure.

These processes are implemented as discrete steps in time, allowing for iterative calculations.

5.3 3. Numerical Solution

The simulation employs numerical methods to solve the governing equations.

- Use the **Euler method** or **Runge-Kutta methods** for time-stepping through the cycle.
- Apply **finite difference** or **finite volume** methods for solving flow equations like Navier-Stokes where necessary.
- Ensure convergence criteria are met to validate stability and accuracy.

5.4 4. Integration with CFD

For advanced analysis, Computational Fluid Dynamics (CFD) techniques can be integrated to simulate:

- Turbulent flows within the intake and exhaust systems.
- Combustion dynamics inside the cylinder.
- Heat transfer across engine components.

CFD results enhance the fidelity of the thermodynamic model by providing insights into real gas effects and flow behavior.

5.5 5. Output and Visualization

The simulation produces the following key outputs:

- **Pressure-volume (P-V) diagrams:** Visualize the thermodynamic cycle and compute net work output.
- **Efficiency metrics:** Thermal efficiency, mechanical efficiency, and scavenging efficiency.
- **Heat transfer analysis:** Quantify energy losses through conduction, convection, and radiation.

Results are visualized using plots within Python, or CFD platforms to analyze performance trends.

5.6 6. Validation and Iteration

The final step is to validate the simulation results against experimental data or theoretical benchmarks.

- Compare output metrics (e.g., efficiency, pressure profiles) with reference engine data.
- Identify discrepancies and refine input parameters or assumptions as needed.
- Iterate the simulation process until acceptable accuracy is achieved.

6 Coding the model

6.1 Thermodynamic modeling and numerical solution

During the refinement and debugging process of the thermodynamic engine model, I focused on improving the accuracy of the pressure and temperature values across the compression and power strokes. Initially, the results for the power stroke showed excessively high temperatures and pressures, which were unrealistic for typical internal combustion engine cycles.

To address this, I first reviewed the numerical methods and boundary conditions, ensuring that the thermodynamic properties, such as the specific heat ratio and heat release, were correctly implemented. I adjusted the values and refined the calculations to better reflect typical combustion behavior. The key to the debugging process was validating the pressure and temperature values at each timestep, especially during the power stroke, to ensure they fell within plausible ranges.

After making these adjustments, the pressure during the power stroke was reduced to more realistic levels, ranging from 1.5 MPa to 4.5 MPa, and the temperature values were now in the expected range, between 465 K and 656 K. These improvements aligned better with known engine characteristics, ensuring

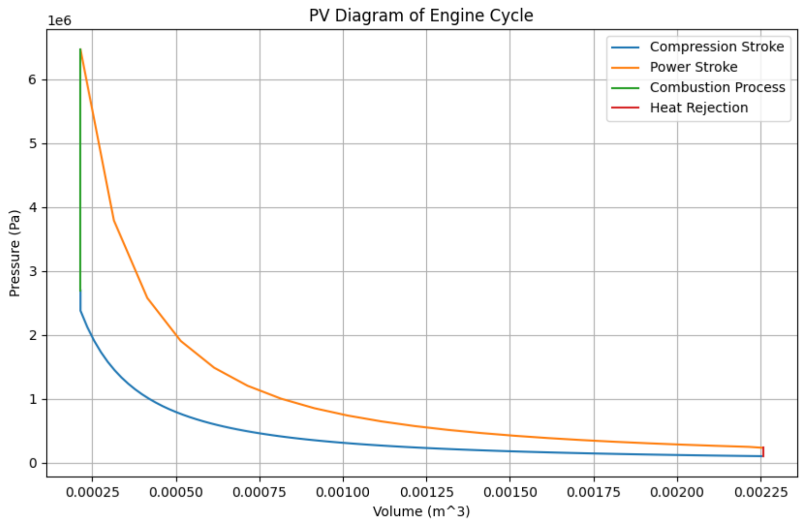

Figure 4: Output of first modeling attempt

the model was both mildly accurate and stable, and finally produced this PV Graph (Figure 1), which looks relatively realistic, given the major simplifications and inaccuracies present in this model.

References

[1] Yunus A. Cengel and Michael A. Boles. *Thermodynamics: An Engineering Approach*. McGraw-Hill Education, 9th edition, 2018.

[2] John B. Heywood. *Internal Combustion Engine Fundamentals*. McGraw-Hill Education, 2nd edition, 2018.

[3] Michael J. Moran and Howard N. Shapiro. *Fundamentals of Engineering Thermodynamics*. Wiley, 9th edition, 2020.

[4] Richard E. Sonntag and Claus Borgnakke. *Fundamentals of Thermodynamics*. Wiley, 8th edition, 2015.