ZHEN-GUO WANG

# INTERNAL COMBUSTION PROCESSES OF LIQUID ROCKET ENGINES

## MODELING AND NUMERICAL SIMULATIONS

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# Preface

Liquid rocket engines are the main propulsion system for a spacecraft. The widespread applications of liquid rocket engines in the future demands further studies of combustion mechanisms in liquid rocket engines to improve their performance. Numerical modeling of the combustion process can improve our understanding of the incorporated physical mechanism and help in the design of liquid rocket engines. Since the 1970s, numerical simulations of combustion in liquid rocket engines have developed into a new interdisciplinary subject involving computational fluid dynamics, computational heat transfer, computational combustion, software design, and flow visualization. Owing to its significance in engine design, this new subject has attracted many researchers. With the rapid development of computer techniques and numerical methods, numerical modeling and simulations of atomization and combustion in liquid rocket engines will become an ever important research area.

The author has dedicated himself to the area of Aeronautical and Astronautical Science and technology since the 1980s. The present book is based on the teaching and supervision of undergraduate and postgraduate students in the past 30 years. The book highlights the advanced research work in the field of combustion modeling in liquid rocket engines, such as liquid propellant atomization, evaporation of liquid droplets, turbulent flows, turbulent combustion, heat transfer, and combustion instability. All these will contribute to our understanding of the combustion mechanism and to the improvement of combustion modeling, facilitating numerical simulations of combustion process in liquid fuelled engines.

The book consists of eight chapters. Chapter 1 describes the configuration and fundamentals of liquid rocket engines, and presents an overview of numerical simulations of combustion in liquid rocket engines. Chapters 2–7 detail the modeling of combustion sub processes in liquid rocket engines, i.e., atomization modeling, evaporation modeling, turbulence modeling, combustion modeling, heat transfer modeling, and combustion instability modeling. Chapter 8 presents a full description of numerical models for combustion, numerical methodology for governing equation solution, and grid generation. Finally, three applications are run to demonstrate the capability of the numerical models to predict the combustion process in liquid rocket engines.

# 1

# Introduction

A liquid rocket engine, which is also called a liquid propellant rocket engine, is a chemical rocket engine using liquid chemicals (liquid propellant) as the energy source and the working fluid. Liquid rocket engine technology has drawn researchers' attention and been quite a hot topic in aerospace and aeronautic research during the last 70 years. In the short long history of human aviation, i.e., from the A-4 engine of the German V2 missile, to the F-1 engine of the U.S. lunar landing rocket "Saturn 5" and further to reusable space shuttle main engines, every milestone event is closely linked with the progress made in liquid rocket engine technology. Because liquid rocket engines have the characteristics of high specific impulse, repeatable starting, arbitrary working hours setting, multiple usage, adjustable thrust, etc., they are bound to occupy the dominant position in the area of aerospace propulsion long into the future.

The liquid rocket engine uses liquid fuels as the propellant. In a liquid rocket engine, the liquid chemical propellants combust in the combustion chamber and produce very high pressure gas. The gas is accelerated when it flows downstream through the nozzle and produces impulse, i.e., thrust, for the aircraft. There are several types of liquid propellants. The scheme, structure, ignition and thermal protection, etc. of the liquid rocket engine have a close relationship with the characteristics of the propellants used by the engine system.

The expansion of liquid rocket application requires more in-depth studies on the basic theory and design method of the liquid rocket engine. Numerical simulation of the combustion process in a liquid rocket engine is also an important research direction. This chapter introduces the basic configuration and working process of liquid rocket engines, and then discusses the main objective and research method of the numerical simulation of the combustion process in a liquid rocket engine.

*Internal Combustion Processes of Liquid Rocket Engines: Modeling and Numerical Simulations*,
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## 1.1 Basic Configuration of Liquid Rocket Engines

A liquid rocket engine consists of a thrust chamber (which consists of an injector, a combustor, and a nozzle), a propellant feed system, propellant tanks and various automatic regulators, etc. This section mainly introduces the propellant feed system and the thrust chambers, which are closely associated with the combustion process.

### *1.1.1 Propellant Feed System*

The propellant feed system is employed to deliver the propellants from the containing tanks to the thrust chamber and can be divided into two categories according to the working mode, namely, the pressure feed system and the turbo-pump feed system.

#### 1.1.1.1 Pressure Feed System

The pressure feed system pushes the propellants to the thrust chamber or the propellant gas generator by the high pressure gas in the tanks of the propellants. The high pressure gas, i.e., the pressed gas, can be pre-stored in cylinders as the storage gas and can also be generated by a liquid or solid gas generator during the working process of the liquid rocket engine. The main requirements for the pressed gas are as follows: (i) high density while under the pressed state, (ii) low relative molecular mass under the pressed state, (iii) minor solubility with propellant, (iv) no or minor chemical reaction with the propellants, and (v) no solid and liquid impurities.

The pressure feed system can employ inert gases as the pressed gas. This kind of pressure feed system has two type of working mode, namely, the regulated pressure mode and the blow-down mode. The former employs a pressure regulator to maintain the pressure in the propellant tank, and also maintains the thrust at a constant value. The latter stores the propellant and the pressed gas in one tank. The pressure drops during the adiabatic expansion of gas, fewer propellants are injected into the combustor and therefore the pressure in the combustion chamber also drops. Typical pressure feed systems are (i) those with high-pressure gas cylinders and (ii) those with gas generators. The former can employ air, nitrogen, helium, and some other inert gas as the pressed gas. The main drawback of air is that the contained oxygen has a relatively high boiling point, and therefore it cannot be used to press cryogenic propellants. Helium can be used to press all existing liquid propellants. Although such a pressure feed system has a relatively large size and heavy mass, it has the characteristics of a simple structure and high reliability. It is also simple to employ and ensures repeatable starting of the engine.

In pressure feed systems with a gas generator, a single-component liquid fuel gas generator using a monopropellant as the source of the driven pressure and the propellant decomposition can be realized by catalysis or heating according to the kind of propellant. In dual-component liquid fuel gas generators, the high pressure gas can be obtained from the two propellant components by burning under oxygen-rich or fuel-rich conditions. The temperature of the gas is determined by the propellant component mixed ratio in the gas generator.

The structure of the pressure feed system is simple and reliable. However, as the propellant tanks must withstand high internal pressure, the pressure feed system is relatively bulky and it is often employed by spacecraft-attitude-control engines. Sometimes, to ensure the reliability of manned flight, although the engine thrust is large, a pressure feed system is also employed, such as the service module engine, drop class, and upgraded engines of Apollo spacecraft.

#### 1.1.1.2 Turbo-Pump Feed System

A turbo-pump feed system employs pumps to deliver propellants, and the pump acquires the driven force from a turbo. In the turbo-pump feed system, a turbo-pump assembly is necessary. The basic requirements for a liquid rocket engine turbo-pump are as follows:

1. If the mass flow rate of a given propellant is given, we need to ensure the pressure at the engine outlet matches the requirement of the engine system.
2. The turbo-pump should be as small and light as possible.
3. The turbo-pump is to have as high an efficiency as possible.
4. The turbo-pump should ensure stable operation at all engine operating conditions and the pressure pulsation and mechanical vibration must be minor.
5. The turbo-pump is to be compatible with corrosive liquid and cryogenic liquids. Friction is not allowed between the components of the oxidizer pump because the heat created by the friction may produce a local high temperature, even an explosion.
6. The turbo-pump is to be capable of sucking propellants that contain a small amount of gas or steam.

There are three common types of cycle program for the turbo-pump feed system, namely, gas generator cycle, expansion cycle, and staged combustion cycle. The gas generator cycle and the staged combustion cycle can employ most of the commonly used liquid propellants. The expansion cycle engine is commonly used in an engine that employs liquid hydrogen as thrust chamber coolant, because liquid hydrogen is a good absorbing-heat medium and it does not decompose.

In the gas generator cycle, the turbine inlet gas is from an independent gas generator, turbine exhaust gas by passing through a small area ratio turbine nozzle, or by injecting in the main stream of the engine through the opening of a nozzle divergence cone. The gas generator propellant can be monopropellant or bipropellant, both of which are from the main propellant feed system. Figure 1.1 shows the bipropellant gas generator cycle turbo-pump feed system; the fuel in the pump portion is injected into the bipropellant gas generator and combust, producing working fluid to drive the turbine. To make sure that the temperature of the combustion products in the gas generator is suitable for the requirements of the turbine, we need to control the propellant mixing ratio in the gas generator, and the gas temperature should be in the range 700–900 °C. Since a bipropellant gas generator system does not require an auxiliary propellant or another tank, its structure is certainly simple, and it is widely employed in liquid rocket engines.

The gas generator cycle is relatively simple. The pressure in the fluid pipes and pumps is relatively low. Therefore, it is the most commonly used turbo-pump cycle. For an engine using the gas generator cycle, the specific impulse of the thrust chamber is slightly higher than that of the engine. However, the thrust of the thrust chamber is always slightly lower than that of the engine.

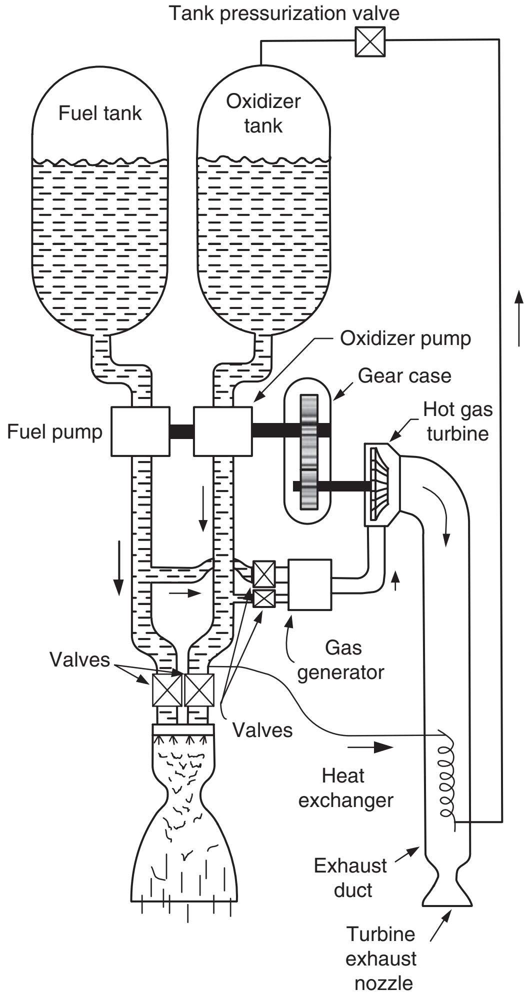


**Figure 1.1** Bipropellant gas generator cycle turbo-pump feed system.

The expander cycle is typically used in an engine that employs liquid hydrogen as the fuel. An expander cycle turbo-pump feed system is shown in Figure 1.2. After absorbing heat from the cooling jacket, the liquid hydrogen becomes heated hydrogen gas. Before entering the main thrust chamber, hydrogen first drives the turbine, and then all the hydrogen gas is injected into the engine combustion chamber, mixed with the oxidant, and combusted. Further, the combustion gas is efficiently expanded in the nozzle and then exhausted. The expansion cycle has high specific impulse. Such an engine is also simple and relatively lightweight. However, the cooling jacket of the liquid hydrogen limits the amount of the absorbed heat, so that the turbine work capability is limited, thereby limiting improvement of the combustion chamber pressure. The pressure in the chamber is generally 7–8 MPa. If the chamber pressure is higher than 8 MPa, this cycle mode is not recommended.

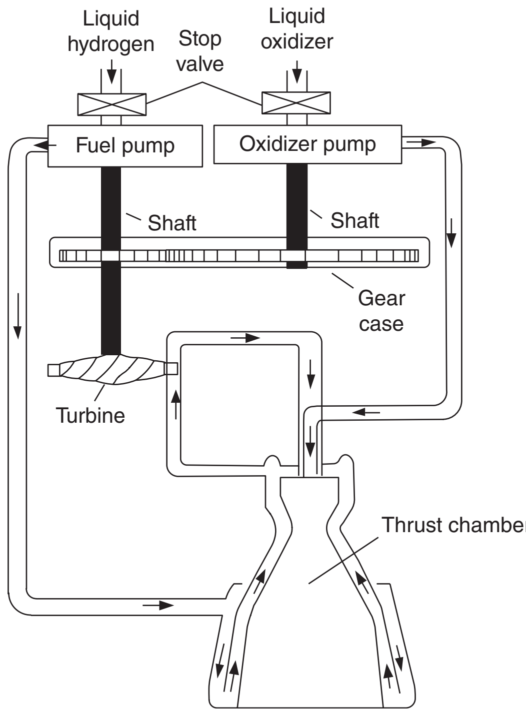


**Figure 1.2** Expander cycle turbo-pump feed system.

Figure 1.3 shows a turbo-pump feed system with staged combustion cycle. In this system, the coolant and fuel firstly flow into a thrust chamber cooling jacket and then are injected into a high pressure pre-combustion chamber where the fuel combusts with part of oxygen. The combustion in the pre-combustion chamber provides the high energy gas for the turbine. After driving the turbine, the gas flows into the main combustion chamber, fully combusts with the oxygen, is exhausted, and is ejected through nozzle.

In a staged combustion cycle, the high pressure pre-combustion can be a monopropellant gas generator or bipropellant gas generator; we can adopt oxygen-rich pre-combustion, such as with the Russian RD120 engine (using liquid oxygen/kerosene propellant) and Russian RD253 engine (using nitrogen tetroxidizer/unsymmetrical dimethylhydrazine propellant). We can also employ fuel-rich pre-combustion such as used in the Space Shuttle Main Engine (using liquid hydrogen/liquid oxygen propellants). Because one of the propellant components goes entirely into the pre-combustion, the flow rate of the turbine working fluid is quite large, so that the turbine output power is greatly improved, and thus a high combustion chamber pressure is allowed to obtain high performance and reduce the size of the thrust chamber. The staged combustion engine has the highest specific impulse; however, the engine is the heaviest and most complex.

In the turbo-pump feed system, the turbine exhaust gas contains energy, and therefore it is possible to improve the specific impulse of the liquid rocket engine through using this energy. If the turbine exhaust gas flows into the liquid rocket engine combustion chamber, where it is

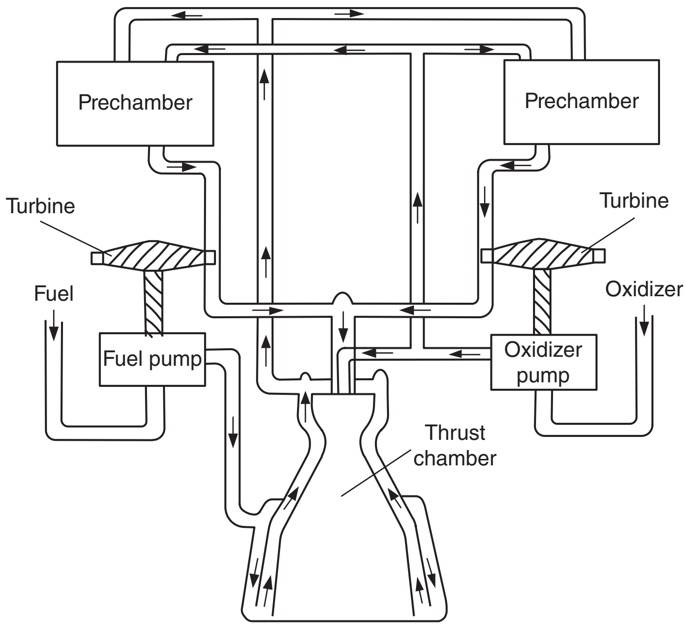


**Figure 1.3** Staged combustion cycle turbo-pump feed system.

combusted with other propellants, this type of pump circulation is called a closed loop. If the turbine gas exhaust goes directly to the surrounding environment or goes into the main flow through the engine nozzle expansion opening section, then this pump circulation is called open cycle. Clearly, the gas generator cycle is an open-cycle, and the expansion cycle and the staged combustion cycle are closed loops. In contrast, an open-cycle engine is relatively simple, operates at low pressure, and the research and development costs are low; however, the closed cycle engine can achieve a higher specific impulse.

### *1.1.2 Thrust Chamber*

A thrust chamber is a device in which chemical energy is turned into mechanical energy. Typically, a device in which chemical energy is converted into heat energy is called a combustion chamber while a device in which heat energy is converted into kinetic energy is called a nozzle. In addition to the combustion chamber and nozzle, a liquid rocket engine thrust chamber also has a unique component—the injector, which is located in the combustion chamber head. Propellant components are injected into the combustion chamber from the injector head, and then they atomize, evaporate, mix with each other, and combust in the combustion chamber. The chemical energy of the propellants is thus converted into heat, producing high-temperature, high-pressure gas. Then, the combustion gas eject from the nozzle at high speed after expansion and acceleration, producing thrust.

Since the thrust chamber works under harsh conditions of high temperature, high pressure, and high flow scour, its structure should satisfy the requirements of high efficiency (combustion efficiency and nozzle efficiency), stable working conditions (reliable ignition start, stable combustion), reliable cooling measures, and good economy (simple structure, light weight, good technology, and low cost), etc.

### 1.1.2.1 Constituents of a Thrust Chamber

***Injectors***

Injectors are usually located in the front of the combustion chamber. The function of the injector is to inject the propellants into the combustion chamber at a fixed flow rate, and let the propellant atomize and mix in a certain ratio to form a homogeneous mixture of fuel and oxidant to facilitate gasification and burning. The injector provides a cooling protective film to prevent the thrust chamber wall from being overheated. In addition, injectors also bear and transfer thrust.

The commonly used injectors can be classified into orifice injectors, swirl injectors, and coaxial tube injectors. Figure 1.4 shows the injector classification.

As shown in Figure 1.5, for an impinging stream pattern, propellant is ejected from numerous independent small holes. The fuel and oxidizer jets then collide with each other, after which a thin liquid fan is produced, which helps the liquid atomize into droplets and helps to produce an even distribution. For a self-impinging stream pattern, oxidizer jets collide with nearby oxidizer jets. Similarly, the fuel jets collide with nearby fuel jets. For a triplet impinging stream pattern, a jet of one component is used to collide with two jets of the other component. When the volume flow rates of the oxidant and fuel are not the same, the triplet impinging stream pattern is more effective.

A shower head stream pattern injector usually employs propellant jet that does not hit and eject from the surface perpendicularly. Mixing is achieved through turbulence and diffusion processes. The engine used in the V-2 missile adopted this kind of injector. A splashed pattern injector helps propellant liquids mix; it applies the principle of a propellant jet impacting with

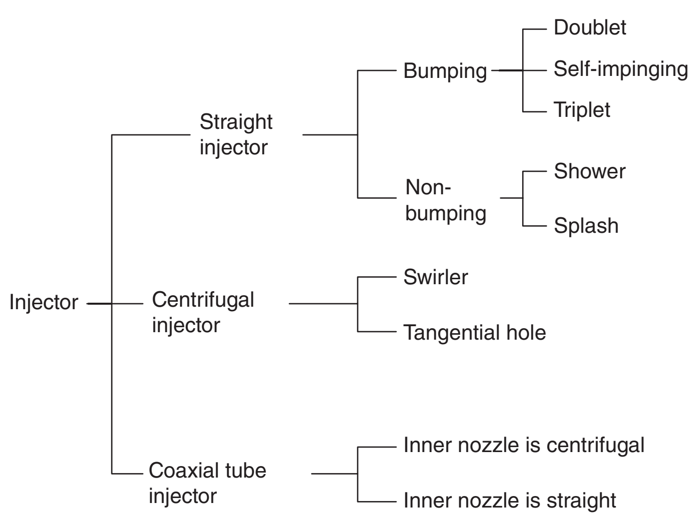


**Figure 1.4** Classification of injectors.

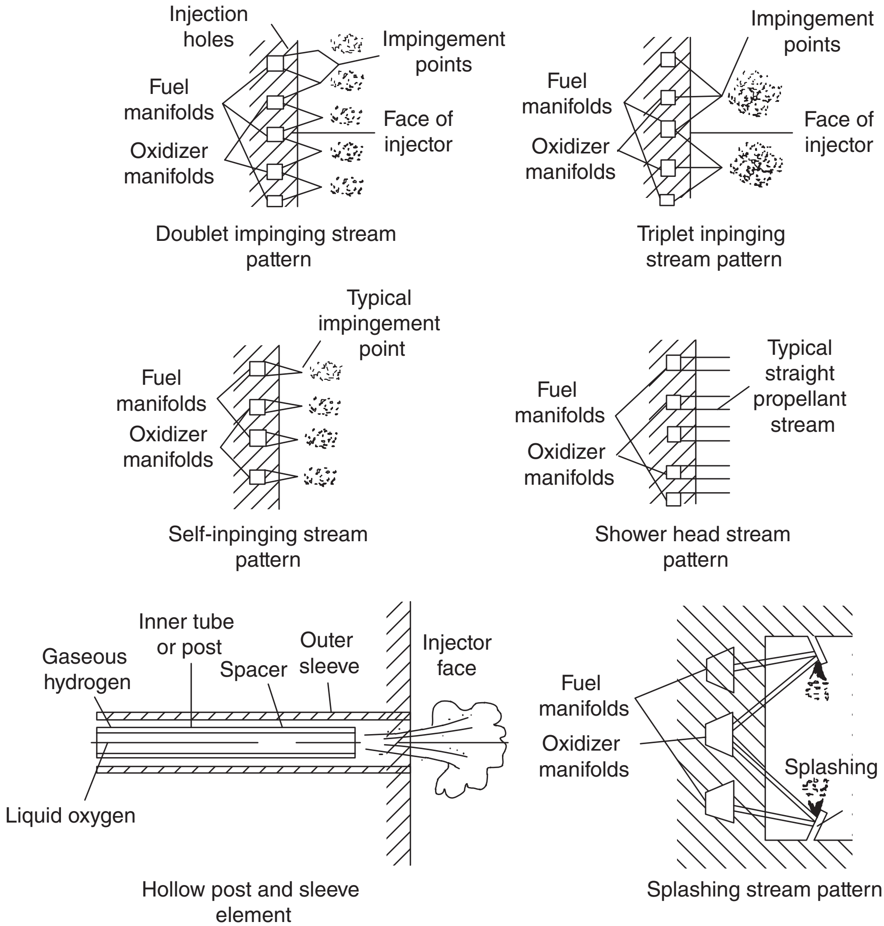


**Figure 1.5** Schematic diagrams of several injector types.

solid surfaces. Certain combinations of propellants that can be stored have successfully used this spraying method. A swirl pattern injector consists of many nozzles as a basic unit; the propellant can be made to form a vortex flow in the nozzle by building a swirler in the nozzle or with drilled tangential holes in the nozzle wall, thus leading to a greater angle cone spray to improve atomization and mixing effect after spraying into the combustion chamber. This injector has a complex structure, large size, but better atomization, and has been widely used. A coaxial tube injector is widely used in liquid oxygen/liquid hydrogen propellant engines. When liquid hydrogen absorbs heat from the cooling channels and vaporizes, this injector is good and effective. Hydrogen gas flows into the chamber along the annular passage, and liquid oxygen flows into the chamber along the cylindrical internal nozzle. The flow rate of the vaporized hydrogen is high, but the oxygen flow rate is low. These differences in flow rate and speed generate a shear force that assists in breaking the liquid oxygen stream into small droplets.

An injector consists of a number of nozzles. There are two basic types of nozzles: swirl injector and orifice injector. Injector performance depends on the structure and properties of the nozzle. It has a great impact on the complete and stable combustion processes of the propellants in the combustion chamber.

***Combustion Chamber***

The combustion chamber is a volume where the atomization, mixture, and combustion processes of the propellants take place. The combustion chamber withstands a high temperature combustion gas pressure, its head is equipped with an injector assembly, and its exit is united with a nozzle. The shape and size of the combustion chamber volume has an important effect on the propellant combustion efficiency. The combustion structure generally is spherical, circular, or cylindrical in shape. A spherical chamber was widely used by liquid rocket engines prior to the 1950s. Although a combustion chamber with this shape has a good bearing capacity, combustion stability, light structural weight, and a small heated area in the same volume, etc., it is rarely employed nowadays because of its structural complexity and difficulties in head nozzle arrangement and processing. The cross-sectional area of the combustion chamber is annular, which was developed to adapt to the so-called plug nozzle and expansion bias nozzle; it has few practical applications. Now the most popular combustion chamber is the cylindrical combustion chamber. This is because it is simple and easy to manufacture, and it is also not expensive to build.

***Nozzle***

As the high-temperature gas in the combustion chamber flows downstream it expands and accelerates in the nozzle, turning the thermal energy into kinetic energy and producing a high-speed jet. The nozzle employed in the rocket engine usually consists of three parts, namely, nozzle convergence region, throat section, and divergent section. Various nozzle cross-sectional configurations are round in the divergent section. Nozzles can be classified as cone-shaped, bell-shaped, plug, and expansion deflection, according to their different longitudinal section. The nozzle should ensure minor total pressure loss of the flow, and the flow at the outlet should be in parallel with the engine axis.

### 1.1.2.2 Cooling of Thrust Chamber

The primary objective of cooling is to prevent the chamber and nozzle walls from being overheated. Once overheated, they will no longer be able to withstand the imposed loads or stresses, thus causing the chamber or nozzle to fail. Basically, there are two cooling methods in common use today, namely, the steady state method and the unsteady state method. For the steady state method, the heat transfer rate and the temperatures of the chambers achieve thermal equilibrium. This includes regenerative cooling and radiation cooling. For the unsteady state method, the thrust chamber does not reach thermal equilibrium, and the temperature of the combustion chamber and nozzle continues to increase in the period of operation. The heat sink cooling and ablative cooling methods are examples of the unsteady cooling method. Film cooling and special insulation are supplementary techniques that are used occasionally with both steady and unsteady cooling methods so as to locally augment their cooling capability. In the following section, we will describe these cooling methods in detail.

***Regenerative Cooling***

In the regenerative cooling method, before the propellant (normally fuel) is injected into the combustion chamber, the propellant flows into the cooling passage that surrounds the combustion chamber for heat exchange through forced convection. The term "regenerative" means that the heat is regenerative. The combustion gas transfers heat to the chamber wall and the wall transfers the heat to the coolant (one propellant component). The heated coolant is injected into the combustion chamber, and this achieves a reuse of the heat energy. This cooling technique is used primarily with bipropellant chambers from medium to large thrust. It has been effective in applications with high chamber pressure and high heat transfer rates. The applications show that the energy loss of this cooling method is trivial. In addition, this cooling method has little impact on the external environment. However, the drawback is its complexity, such as the complex structure of the cooling passage of the thrust chamber. Furthermore, the flow in the cooling passage brings hydraulic loss.

For a thrust chamber using regenerative cooling, the structural strength of the whole thrust chamber, the cooling reliability, and the structure mass, etc., are closely related to the structure of the cooling passages. Popular thrust chamber cooling passage structures of regenerative cooling systems are mainly as follows:

1. A smooth slit pattern cooling passage formed between the inner and outer walls:
   The structure of the smooth slit pattern cooling passage formed between the inner and outer walls is simple (Figure 1.6). However, in the case of a small flow of cooling liquid, to ensure the desired flow rate, the channel gap size must be small (<0.4–0.5 mm), which is difficult to achieve in the manufacturing process. Further, when the pressure in the cooling passage is high, the thin inner wall can easily deform as it is not rigid enough.
2. A cooling passage of inner and outer walls connected to each other:
   There are three main forms of this type of passage. One form is produced by welding the inner and outer walls together in the special punching holes (Figure 1.7). The holes are

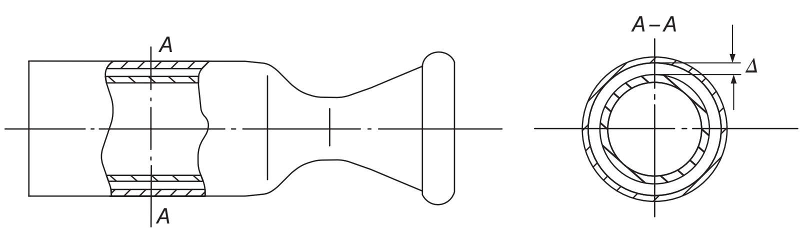


**Figure 1.6** Schematic of a smooth slit pattern cooling passage.

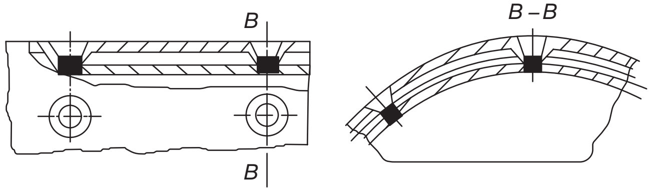


**Figure 1.7** Schematic of connected cooling passage at the indentation.

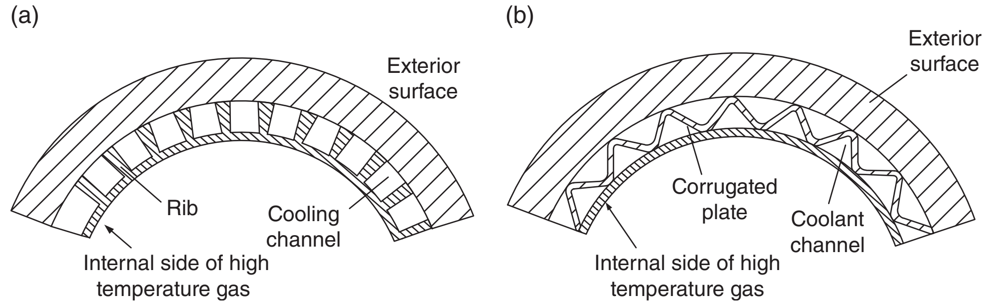


**Figure 1.8** Schematic of brazed inner and outer wall of a cooling passage: (a) solder along the outer edge of the ribs; (b) solder along the inner and outer walls of the corrugated boards.

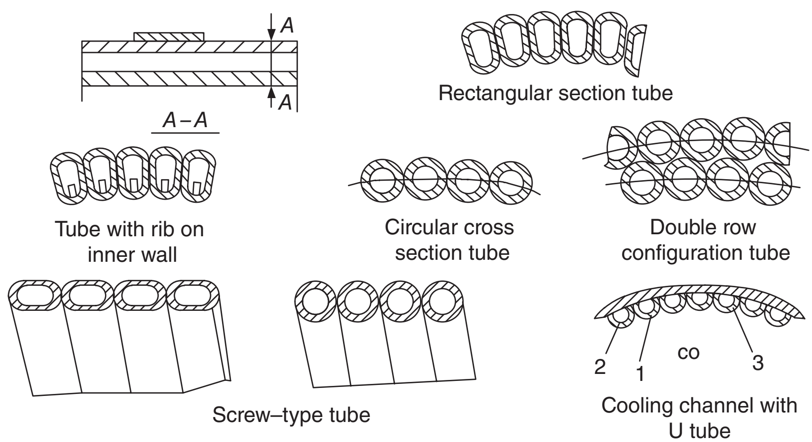


**Figure 1.9** Tube bundle cooling passage.

located in the outer wall, and their shape can be circular or elliptical. Another form is produced by soldering the outer wall with the ribs milled on the inner wall (Figure 1.8a); the third form is obtained by inserting a corrugated plate and solder along the inner and outer walls of the corrugated plate (Figure 1.8b).

3. Tube bundle cooling passage:

   Engines manufactured in the United States of America widely adopt the thrust chamber tube bundle structure shown in Figure 1.9. This kind of thrust chamber body part is combined by special tubules (0.3–0.4 mm) with certain types of surface. Tubules are made of materials with good heat transfer performance (generally nickel alloy), and are soldered together. To ensure the strength of the tube bundle type thrust chamber we should use special enhancement techniques, for example, installment of staged reinforcing ring and use of entire bearing coat.

***Radiation Cooling***

When using radiation cooling, the thrust wall is a single layer wall made of refractory metal, such as molybdenum, tantalum, tungsten, and copper alloy, and heat radiates directly from the outside surface of the thrust chamber. The cooling capacity of the radiation cooling depends on the temperature of the thrust chamber and the surface characteristics of the thrust chamber. The radiation energy ($E$) is a function of the fourth power of the absolute temperature ($T$), i.e.:

$$E = f\varepsilon\sigma A T^4 \tag{1.1}$$

where:

$f$ is a geometric factor that is determined by the relative position and shape of near objects;
$\varepsilon$ is the blackness, which is a dimensionless coefficient determined by the surface condition and the material properties;
$\sigma$ is the Boltzmann constant $\left(1.38 \times 10^{-23}\,\mathrm{JK}^{-1}\right)$;
$A$ is the surface area.

Radiation cooling is a simple cooling method whose construction weight is light; it is widely used in low temperature gas engines, e.g., monopropellant hydrazine engines used in aircraft maneuver and attitude control, and the maximum temperature of the combustion chamber is only about 850 K. This cooling method is also widely used in the gas generator chamber, the nozzle outlet and the extension or skirt section of the nozzle exit. To reach the requested heat flux, a high temperature of the metal wall is necessary.

***Heat Sink Cooling***

When using heat sink cooling, the thrust chamber is a non-cooling, heavy, metal structure and its wall is very thick. During operation, heat is absorbed sufficiently by the heavy wall before it reaches a temperature that would cause damage. Therefore, the heat-absorbing capacity of the thrust chamber wall material determines the longest operation period of the thrust chamber. This method is mainly used in the case of a low pressure chamber and low heat transfer rate, such as with the heavier experimental engine.

Cooling methods also include ablative cooling, film cooling, and special insulation cooling. When using ablative cooling, the thrust wall is made of ablative materials (typically resin materials). At temperatures of 650–800 K, ablative materials absorb heat and decompose into a porous carbonaceous layer and pyrolysis gas, and the gas forms a fuel-rich protective boundary layer on the carbon surface. Film cooling makes use of various measures (such as a dedicated head cooling jet orifice, holes and slots forming the films on the walls, a wall made up of porous material) to inject the liquid propellant component or cool air. A liquid layer and its vapor film form on the inner wall of the chamber to isolate the burned gas, reducing the wall temperature. The special insulation method adopts refractory metal and refractory material as the coating to improve the allowed upper temperature limit of the wall and reduce the heat flux to the chamber walls.

## 1.2 Internal Combustion Processes of Liquid Rocket Engines

Liquid rocket engine operation characteristics include performance, stability, and compatibility. Actual specific impulse is used to evaluate performance. Stability refers to an engine combustion process that does not produce any instability, it is measured using dynamic stability indicators. Compatibility refers to the ability of the thrust chamber wall to withstand high temperature and high pressure gas; it is described by the ability of the thrust chamber wall and propellant to work compatibly. Performance, stability, and compatibility are three key issues to be solved in the development of liquid rocket engine. Since these tissues are correlated, the possibility of finding a comprehensive solution to meet all three requirements should be explored to improve the combustion process. This section briefly describes the working process of a liquid rocket engine and then introduces the combustion process.

### *1.2.1 Start and Shutdown*

The process involved from sending a starting instruction to establishment of the primary working condition is called the start. During the start, the engine goes through a series of procedures and related processes to ensure the transition from starting preparation state to primary working condition state. During the startup, there are unstable processes in the combustion chamber and engine equipment; the flow conditions of these processes will determine the reliability and performance of a liquid rocket engine. For example, so-called water hammer occurring at startup can destroy a liquid rocket engine's rated working condition, and even cause engine damage. Therefore, it is important to ensure a reliable engine start, as most liquid rocket engine failures occur during the start.

Usually, liquid rocket engines need to complete the following processes at startup: the pressure in the propellant tank first increases to the specific pressure; for liquid rocket engines using cryogenic propellant, it is necessary to cool the propellant lines; the propellant feed system (e.g. turbo-pump) goes into the specified working state; for liquid rocket engines using non-hypergolic propellant, the initial ignition flame should be produced in the thrust chamber and gas generator to ensure ignition of the propellant injected into the thrust chamber and gas generator; the propellant valve should be opened to ensure the propellants eject into the combustion chamber and gas generator.

The operations listed above are typical, but some of them are not necessary for certain types of liquid rocket engines and some operations are not needed according to special requirements. In turbopump-fed liquid propellant rocket engines, the schemes of turbine start can be classified into self-start and external-energy start according to the way the energy needed is provided. Self-start does not require additional boot devices. External energy start schemes include gunpowder start (use gunpowder-generated gas to drive turbine) and cylinder start (use of bottled pressed gas to drive the turbine).

The transition process from sending shutdown instructions to the thrust dropping to zero is called the liquid rocket engine shutdown. Engine shutdown is necessary. For example, we need to shut down engines when the rocket reaches the desired speed, the spacecraft complete the necessary maneuvers, and experiments are completed or fail on the test bench. Shutdown methods and various operations depend on the requirements of a liquid rocket engine, and these requirements depend on working conditions and aircraft functions.

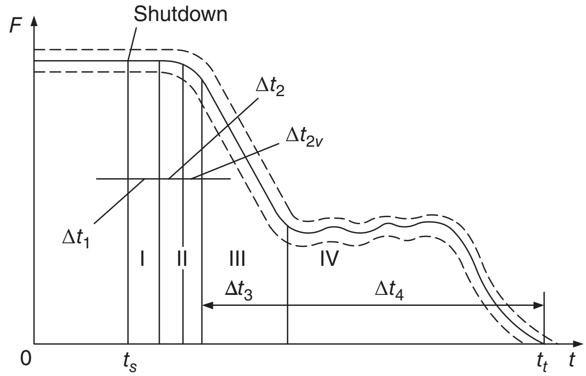


**Figure 1.10** Typical thrust attenuation characteristics at shutdown.

According to different requirements proposed for a rocket system, the shutdown method can be divided into the following modes: shutdown after propellant consumption, shutdown guaranteeing minimum aftereffect impulse, fault shutdown, and multiple-shutdown. A working liquid rocket engine on an aircraft in active flight usually adopts the first shutdown method, e.g., shutdown of the liquid rocket engine on ballistic missiles.

The difference between shutdown guaranteeing minimum aftereffect impulse and the first shutdown is that for a given case the former makes an additional requirement that a minimum aftereffect impulse should be ensured. The so-called impulse is thrust impulse produced in the period from sending the shutdown instruction to the thrust dropping to zero. Figure 1.10 shows typical thrust attenuation characteristics during the shutdown. First, from sending the shutdown instruction to the main valve being turned off, the propellant injected into the combustion chamber has to be delayed for a certain time to change into combustion gas, namely, there is a combustion delay $\Delta t_1$, so the whole process moves to the right along the time axis, and the thrust remains unchanged. Secondly, after sending the shutdown instruction, the valve needs the time $\Delta t_2$ to operate due to the inertia of the control circuit, when the propellant flow and thrust remain unchanged. After $\Delta t_2$, the valve begins to close, and when the flow cross-sectional area begins to change, the thrust and flow also change. Because of the inertia of the valve it needs the time $\Delta t_{2v}$ to shut down completely. After the valve is closed completely, the gas in the combustion chamber disappears quickly, the pressure in the combustion chamber declines sharply; the time taken for this process is $\Delta t_3$. The evaporation and combustion of residual propellants corresponding to $\Delta t_4$ in Figure 1.10 is determined by the unstable process by which the remaining propellant from the main valve to the injector head cavity flows into the combustion chamber. When the chamber pressure drops below the propellant component saturation vapor pressure, the propellant in the head cavity is injected into the combustion chamber under the saturated vapor pressure effect. Due to the difference between the two component saturated vapor pressures, the first entering the combustion chamber evaporates first and discharges, leading to partial thrust; When both components have entered the combustion chamber, combustion occurs. At this stage, the mixed ratio in the combustion chamber is changing, often deviating from the optimum value, and the combustion is unstable. Shutdown failure happens easily. Since the process is in a non-controlled state, it directly affects the aftereffect impulse deviation. The aftereffect impulse can be reduced by adopting the staged shutdown method which reduces the thrust during shutdown, or by shorting the pipeline, reducing the valve actuation time and reducing the residual volume of the residual propellant. We can also force to empty the residual propellant to mitigate the aftereffect impulse.

Multiple shutdown and startup of liquid rocket engines are used in orbiter aircraft and aircraft that need to start periodically. To achieve multiple shutdowns, liquid rocket engines must be able to automatically transit to the state that startup preparation is completed; consequently, most multiple-shutdown liquid rocket engines use the same equipment to complete the startup and shutdown.

### *1.2.2 Combustion Process*

The combustion process of liquid propellant is a very complex process from the injection of liquid propellants to formation of the combustion products. The internal combustion process in a liquid rocket engine might be the most complicated combustion and flow phenomena. This is mainly because (i) the combustion process in a liquid rocket engine actually contains many physical/chemical sub-processes of several types, multiple characteristics, and different temporal and spatial scales. Whether these sub-processes can be simulated using a specific model is highly dependent on the propellants and rocket engines. (ii) Generally, many sub-processes occur simultaneously and are strongly coupled. It is usually very difficult to decouple these into independent processes. (iii) The propellant mass flow rate in the combustion chamber can reach hundreds or even thousands of kilos per second while the residence time of propellants in the combustion chamber is very short at the order of several milliseconds. But, the combustion efficiency requirement is very demanding, up to 0.98–0.99. (iv) In the combustion chamber, the propellant concentration gradient, temperature gradient, and pressure gradient are significantly high in the vicinity of injectors. Therefore, the flowfield is very complicated. Furthermore, the pressure, velocity, and temperature in the combustion chamber of rocket engines are much higher than in other engines (e.g., jet engines), which induces more difficulties for combustion. (v) Combustion instability of different frequencies is prone to occur, which may cause a performance reduction and damage to the facility.

Figure 1.11 presents the individual sub-processes of spray combustion in a liquid rocket engine. These sub-processes occur in the two-phase flow in the combustion chamber.

Based on available experimental results, the flowfield can be qualitatively divided into a series of discrete zones (Figure 1.12):

1. Injection–atomization zone:

   The injected propellant mainly atomizes and forms liquid drops in this zone. Since the liquid fuel and oxidizer are sprayed independently through different injectors and inject into the combustion chamber via the orifices with a certain distribution and orientation, the mass flux, mixing ratio, atomization performance, and the properties of the gases varies significantly in different directions, which consequently leads to a mixing process. The majority of the gas in the injection–atomization zone is the gaseous propellant component or the recirculated combustion gas from the downstream. The recirculation of combustion gas is mainly caused by the shear stress between the propellant jet and the surrounding gas. This shear stress also twists the jet surface and causes jet breakup, which is helpful for atomization. Gas–liquid injectors are designed according to the atomization mode caused by shear stress

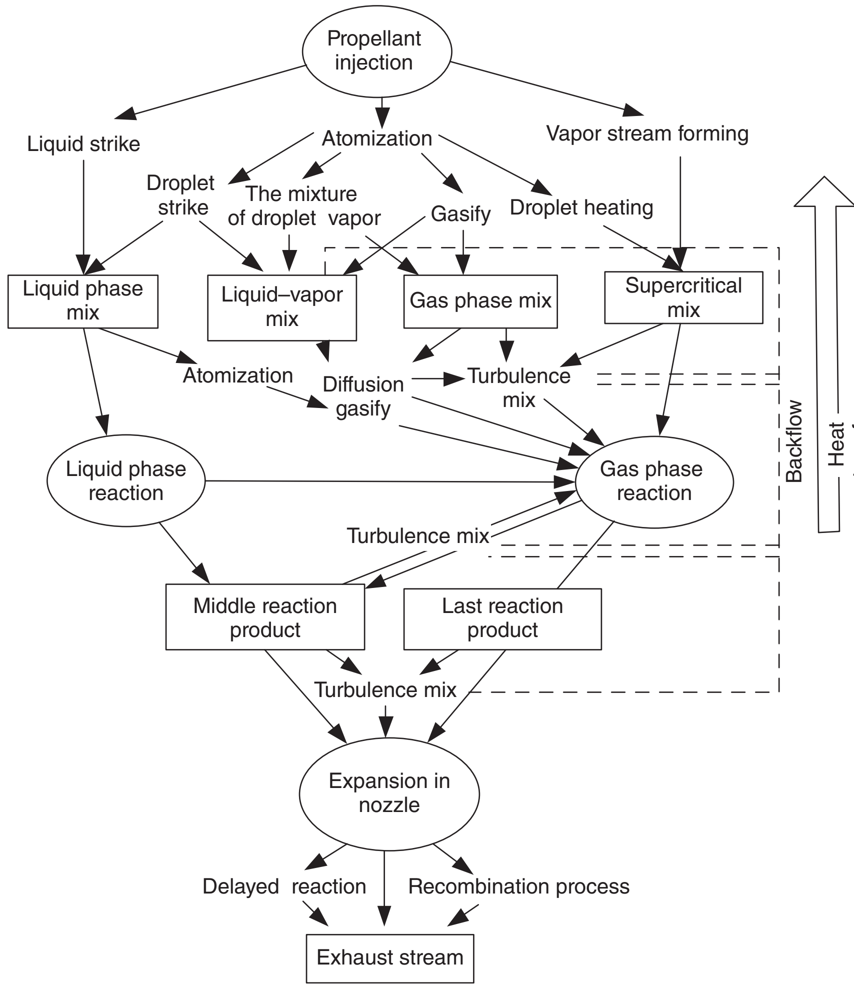


**Figure 1.11** Schematic of internal combustion process in a liquid rocket engine.

breakup. However, for most of the liquid–liquid injectors, atomization is usually achieved using liquid jet impingement or swirl injectors. The accomplishment of atomization needs a certain distance, usually 1–5 cm. The formation and distribution of liquid drops proceeds simultaneously. Once liquid drops form, they are surrounded by the gases. The temperature of the surrounding gas is higher than that of the liquid drops and therefore the liquid drops are heated. Since the initial temperature of the liquid drops is significantly lower than the propellant saturation temperature under the thrust chamber pressure, the vaporization of propellants in this zone can be neglected. As the temperature of the liquid drops and surrounding gas elevates, the vaporization rate keeps increasing, and chemical reactions between the fuel vapor and oxidizer vapor start, with transfer to the next zone.

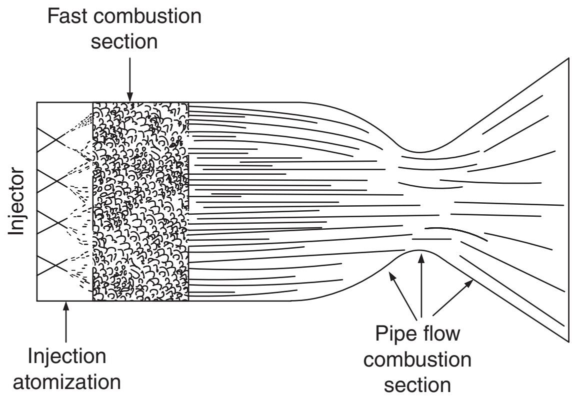


**Figure 1.12** Schematic of zone division of combustion process in a liquid rocket engine.

2. Rapid combustion zone:

   The characteristic of this zone is that the propellant jet has completely become a liquid mist, which vaporizes quickly, mixes, and reacts to produce combustion products. Although the spray diffusion and flow recirculation reduces the transverse gradient of flow parameters in the injection–atomization zone, it still cannot be neglected for most liquid rocket engines. Therefore, the mass, heat, and momentum exchange in radial and circumferential directions, leading to the acceleration of mixing and evaporation processes. As a result, the combustion products are quickly produced, which leads to gas acceleration dominantly in axial direction and also causes transverse flow from the high combustion rate zone to the low combustion zone and recirculation of combustion gas to the injection–atomization zone.
3. Stream tube combustion zone:

   The transverse movement of atomization and combustion gas almost disappears. The evaporation and combustion occur in stream tubes parallel to the engine axis. In addition, the mixing between stream tubes relies on turbulent oscillation. Since the velocity of a combustible gas is high, the residence time of propellant in the combustion chamber is about 3–5 ms. Given that the turbulent oscillation frequency is about 1000–2000 Hz, turbulent fluctuation occurs in the combustion chamber no more than ten times and, thus, turbulent exchange is not significant. High-speed photography shows that the flow in this zone is close to laminar flow. As the distance from injection plate increases, the local residence time decreases and the relative velocity between droplet and gas flow decreases. The stream tube combustion zone then ends at the sonic section of the nozzle.
4. Supersonic expansion zone:

   As the expansion of combustion products continues in the nozzle, the vaporization and combustion can be assumed to stop as status parameters such as the pressure and temperature decrease and the residence time minimizes. The loss of energy in the supersonic zone in the nozzle should be linked to the two-dimensional nozzle flow, boundary layer loss, and the chemical hysteresis of the combustion products decomposition.

### 1.2.3 Performance Parameters in Working Process

The rocket engine performance parameters (e.g., total impulse, specific impulse, and the mixture ratio) are defined in this section.

The total impulse of a rocket engine can be defined as the integration of thrust ($P$, which is time-dependent) over the entire combustion time, $t$:

$$I_t = \int_0^t P\,\mathrm{d}t \tag{1.2}$$

The total impulse is a very important performance parameter. Since it contains the thrust and its duration, it represents the level of engine's working capability.

The specific impulse is the impulse produced by burning 1 kg of propellant in a rocket engine:

$$I_\mathrm{s} = \frac{I_t}{m_\mathrm{p}} \tag{1.3}$$

where $m_\mathrm{p}$ is the total effective propellant mass and $I_\mathrm{s}$ is the average specific impulse in the operation process.

For liquid rocket engines, the specific impulse is the thrust generated by consuming 1 kg propellant per second:

$$I_\mathrm{s} = \frac{P}{\dot{m}} \tag{1.4}$$

The specific impulse is an important performance parameter that has a significant influence on the performance of space launchers and spacecrafts.

The density specific impulse is defined as the thrust generated by a unity of propellant mass flowrate:

$$I_{\mathrm{s,p}} = \frac{P}{\dot{V}} = \frac{P}{\dot{m}/\rho_T} = I_\mathrm{s}\rho_T \tag{1.5}$$

where $\rho_T$ is the density of propellant.

The mixture ratio of propellant is defined as the ratio of oxidizer mass flow rate to the fuel mass flow rate:

$$\mathrm{MR} = \frac{\dot{m}_\mathrm{o}}{\dot{m}_\mathrm{f}} \tag{1.6}$$

MR has a significant effect on the specific impulse of a rocket engine. It also influences the propellant density ($\rho_T$) and thus has a strong effect on the structure, mass, and dimensions of rockets and spacecrafts and further on the performance of the launchers.

## 1.3 Characteristics and Development History of Numerical Simulation of the Combustion Process in Liquid Rocket Engines

### *1.3.1 Benefits of Numerical Simulation of the Combustion Process in Liquid Rocket Engines*

1. Shortening of the development period and reduction of research cost:
   The complexity of the operation process of a liquid rocket engine means that the calculations show significant discrepancy in comparison with practical testing results. For a long period, the design and development of a rocket engine relied on experiments. It has to go through many specific and full-scale engine tests, resulting in huge costs and long research periods. Numerical calculation of the combustion process in a liquid rocket engine can reproduce the practical combustion process on a computer. The unreasonable testing schemes can be abandoned based on simulation results. This can significantly reduce the number of tests and increase the testing success rate. The overall research period can be shortened and research costs can be reduced. Additionally, numerical simulations of liquid rocket engine combustion can help researchers perform quick design optimization and complex calculations.
2. Detection of potential problems and prediction of engine performance:
   During the operation process in liquid rocket engines, the high-temperature and high-pressure combustion gases pose a demanding environment for most testing instruments. The experimental data measured from one test is limited and is not enough to analyze experimental phenomenon. However, numerical simulations can provide a large amount of combustion process information, which can be used to help identify the cause of experimental phenomenon and provide clues for solving the problem. As the numerical simulation technique develops, it can precisely predict the complicated working process and performance in engines. The carrying out of numerical simulations will allow researchers to estimate the performance before hot-fire tests and will be beneficial in results analysis and performance evaluation after hot-fire tests. The numerical simulation results are completely repeatable, which can allow researchers to observe the work process at any stage and conduct quantitative studies. From this viewpoint, numerical simulations of the combustion process in liquid rocket engines are a kind of hot-fire tests on computers using a numerical method.

### *1.3.2 Main Contents of Numerical Simulations of Liquid Rocket Engine Operating Process*

As mentioned above, the combustion process in a liquid rocket engine is a combustion and flow process with complex boundary conditions. The main parameters of a liquid rocket engine are determined by the flow and combustion process. However, combustion instability may cause structure failure of engines, which may also be related to the combustible gas flow process. Therefore, it can said that the numerical simulation of combustible gas flow and combustion process is the key problem in the numerical simulation of the combustion process:

1. Modeling of combustion process:
   The internal flow in liquid rocket engines can be described by three-dimensional unsteady compressible Navier–Stokes equations. The effect of two-phase flow, chemical reaction,

heat convection, heat radiation should be taken into account. Generally, the combustible gas flow in a combustion chamber has three-dimensional characteristics. In addition, this three-dimensional effect will affect the combustion gas flow in the nozzle.

Numerical models of the combustion process in liquid rocket engines contain an atomization model, liquid droplet evaporation model, flow turbulence model, combustion model, and heat transfer model. Since the flow, combustion, and heat transfer processes are coupled, these models are inter-related. The spray and combustion of liquid propellant is a complicated process containing heat transfer, fluid movement, mass and concentration diffusion, and other chemical dynamic processes. Therefore, it is very difficult to set up a comprehensive theoretical model. In liquid rocket engines, the flow of combustion gas is turbulent. Turbulence simulation usually applies Reynold average equations with turbulence models to enclose the equations. However, there is no turbulence model that can work at all conditions. Numerical simulations of internal flow in engines have to properly deal with the droplet distribution, droplet velocity and thermal properties of further formed two-phase mixture, particles dynamics and energy characteristics, physical properties of particle state, and size distribution. Liquid droplet evaporation is influenced by high pressure, multiple species, and pressure oscillation. A proper model describing this process should be developed. Heat transfer in liquid rocket engines occurs in three fundamental ways, namely, heat conduction, heat convection, and heat radiation

Generally, the main ways heat transfer takes place in liquid rocket engines are heat convection and heat radiation with even higher heat convection. The energy conservation equation with heat radiation is an integral–differential equation, which is very complicated to solve especially in the calculation of spatial angle coefficients. The physical properties of radiation heat transfer are not easy to determine in liquid rocket engines when considering temperature and pressure variations. Combustion instability is an unsteady phenomenon occurring in liquid rocket engine combustion. The most common form is periodic combustion oscillation.

Combustion oscillation can occur spontaneously, and often appears at a specific characteristic time in the combustion process. This characteristic time is determined not only by the combustor geometry but is also related to gas flow variation. When variations go beyond the system stable limit, the flow turbulence is amplified by the interaction of combustion and average flow, which can lead to severe damage. Modeling of combustion instability is very difficult but some progress has been made.

2. Solution of Numerical Model

Numerical simulation of the combustion process in liquid rocket engines relies on solving governing equations including combustion and heat transfer models with complex boundary conditions. Consequently, numerical solution of simulation models becomes a key point where the computation of heat transfer and combustion is also required. Computational fluid dynamics is a new subject, arising with the development of computer science and technology. The discretization method has three schemes: finite difference, finite element, and finite volume. Numerical schemes of temporal discretization can be divided into three categories: explicit, implicit, and explicit–implicit. Every scheme contains first- and second-order resolution schemes and other high-order schemes developed in recent years. For numerical simulation of flow field, the selection of discretization methods and numerical schemes depends on the governing equations, solution scales, requirements of numerical solution, computation efficiency and accuracy, and the available computer resources.

The numerical solution process in computational fluid dynamics can be generally divided into three procedures:

1. pre-processing, including model setup, division of simulation domain, and grid generation;
2. numerical solution, containing scheme selection, equation discretization, initialization, boundary condition specification, coding and debugging, and computation;
3. post-processing, involving visualization of flow properties using numerical methods and flowfield analysis.

3. Analysis of simulation results:

After completion of numerical simulations, the analysis and study of the operation process of rocket engines can be carried out using various methods. With the help of image flow visualization techniques, the internal flow structures, flow processes, combustion process, and their interaction can be investigated in detail to predict engine performance.

### *1.3.3 Development of Numerical Simulations of Combustion Process in Liquid Rocket Engines*

To maintain high reliability and reduce the test cost of liquid rocket engine design, usually several modifications are made to the current engine design based on engineering experience. Then these design modifications are evaluated using a large number of tests. However, the engine tests are always expensive and time-consuming. A single engine test may cost tens of thousands, hundreds of thousands, and even several million RMB Yuan. The measurement and diagnostics are also very challenging because of the high temperature and pressure in the combustion chamber and their rapid variation. It is very difficult to obtain enough reliable measurement data, accurate performance improvement, and the cause of failure. Therefore, the design of combustion chambers, especially injectors, is the most time-consuming period in the development of a liquid rocket engine.

To avoid the reliance of liquid rocket engine design on pure experience, the Chemical Rocket Propulsion Cooperation Bureau and Performance Standardize Team was founded for this work in the USA in 1965. It published an assessment guidance for liquid rocket engines. The guidance presents all the performance losses except the energy release (combustion process) loss. As the combustion process was believed to be too complicated to describe using analytical methods, it was supposed that propellants burn completely and the propellant enthalpy is reduced to account for this effect in the calculation of heat equilibrium. These approaches all show difficulties in numerical simulations of the combustion process. In the 1970s, as combustion computation developed, the computation techniques were applied to liquid rocket engine design. Many combustion computation models were developed for specific newly designed engine prototypes in the 1980s, such as the combustion computation model for the combustion chamber design of auto-ignition liquid rocket engines F-20 and F-5, the ARICC model for the injector/combustion chamber of space shuttles and advanced rockets, PHEDRE model for Ariane rocket engines, REFLAN3D-SPRAY model for liquid oxygen/hydrocarbon rocket engines, and CAFILRE code for liquid hydrogen/liquid oxygen rocket engines. In the 1980–1990s, most books in China on liquid rocket engines still focused on the introduction of thermal calculation, and aerodynamic and heat transfer calculation. For example, Professor

Fengchen Zhuang published the book *The Theories, Models and Applications of Liquid-Propellant Rocket Engine Spray Combustion* [1].

Another issue to solve in the combustion simulation of liquid rocket engines is the turbulent two phase flow and combustion process using full Navier–Stokes equations. To further improve the numerical accuracy of models and understand more details (temperature distribution, concentration distribution, velocity distribution, and pressure distribution) of the entire flow field in the combustion process from start to shutdown, a more complicated model covering all combustion sub-processes should be developed. These models and programs have improved applications of liquid rocket engine atomization models. The author of this book has conducted much work in liquid rocket engine research and development [2–7]. This book is a summary of work conducted in recent years.

Numerical modeling of combustion process in liquid rocket engines has been a multidisciplinary subject since the 1970s. It combines computational fluid dynamics, computational heat transfer, computational combustion, computer software design, and flow visualization. Therefore, it is one of the most active research subjects in the liquid rocket engine research field. The numerical simulation of liquid rocket engine working processes has been applied in every aspect of liquid rocket engine research. It is an efficient research method, and also can assist the design and experimental study. Therefore, further development of this research subject can significantly improve understanding of fundamental physical phenomena and the engine design.

## 1.4 Governing Equations of Chemical Fluid Dynamics

Combustion is a flow process containing chemical reactions. No matter how complex the combustion processes are they all obey the fundamental laws of nature, namely, the conservation of mass, species, momentum, and energy. The mathematical equations representing these laws are from chemical fluid mechanics, also referred to as the fundamental governing equations of a combustion process. These equations are the fundamentals of numerical simulations of the combustion process. They will be presented in the following and the physical meaning of these equations is briefly described. For the mathematical expression of multidimensional variables, the tensor notation is applied. Subscriptions $i$, $j$, $k$ indicate the coordinate direction. The variables with only one subscription are vectors, e.g., $u_i$. Variables with two subscriptions are tensors, such as viscous stress $\tau_{ij}$. The same subscription appearing twice for a variable indicates Einstein's summation convention of this variable from index 1 to 3.

In Cartesian coordinates, the governing equations contain the following four equations:

1. Continuity equation:

$$\frac{\partial \rho}{\partial t}+\frac{\partial \rho u_i}{\partial x_i}=0 \tag{1.7}$$

2. Momentum equation:

$$\frac{\partial \rho u_i}{\partial t}+\frac{\partial \rho u_i u_j}{\partial x_j}=\frac{\partial p}{\partial x_i}+\frac{\partial \tau_{ij}}{\partial x_j}+g_i-f_i \tag{1.8}$$

where $\rho$ is the density of the fluid mixture; $p$ is the pressure; $u_i$ is the velocity in the $i$ direction; $g_i$ and $f_i$ are the components of gravity and other drag in the $i$ direction, respectively; $\tau_{ij}$ is the viscous stress tensor, which can be related to strain rate tensor $S_{ij}$ using generalized Newton's law:

$$\tau_{ij} = 2\mu S_{ij} - \frac{2}{3}\mu S_{kk}\delta_{ij} \tag{1.9}$$

$$S_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) \tag{1.10}$$

where $S_{kk}$ is the fluid volumetric dilatation $div\mathbf{u}$, which represents the volumetric expansion and compression; $\mu$ denotes the fluid dynamic viscosity coefficient; $\delta_{ij}$ is the second order unit sensor, if $i = j$, $\delta_{ij} = 1$; otherwise $i \neq j$, $\delta_{ij} = 0$.

3. Energy equation:

$$\frac{\partial \rho h_0}{\partial t} + \frac{\partial \rho u h_0}{\partial x_j} = \frac{\partial}{\partial x_j}\left(u_i \tau_{ij}\right) + \frac{\partial}{\partial x_j}\left(\lambda \frac{\partial T}{\partial x_j}\right) + \rho q_{\mathrm{R}} + \frac{\partial}{\partial x_j}\left[\sum_l \left(\Gamma_l - \Gamma_h\right)\frac{\partial m_l}{\partial x_j}\right] \tag{1.11}$$

where $h_0$ is the stagnation enthalpy, also the total enthalpy, $h_0 = h + u_i u_1/2$, $h = \sum_l m_l h_l$, $m_l$ and $h_1$ are the mass fraction and specific enthalpy of specie $l$ in the fluid mixture; $\Gamma_l$ and $\Gamma_h$ are the transportation coefficient of specie $l$ and exchange coefficient of enthalpy; $q_{\mathrm{R}}$ is the radiant heat flux. If using the definition of total enthalpy, $T$ in the diffusion term on the right-hand side of Equation 1.11 can be replaced by $h_0$. Therefore, we can get an alternative form of the energy equation:

$$\frac{\partial \rho h_0}{\partial t} + \frac{\partial \rho u_j h_0}{\partial x_j} = \frac{\partial}{\partial x_j}\left(\Gamma_h \frac{\partial h_0}{\partial x_j}\right) + S_k \tag{1.12}$$

where the source term is:

$$S_k = \frac{\partial p}{\partial t} + \frac{\partial}{\partial x_j}\left(u_i \tau_{ij}\right) + \rho q_{\mathrm{R}} + \frac{\partial}{\partial x_j}\left[\left(\lambda - \sum_l m_l c_{pl} \Gamma_k\right)\frac{\partial T}{\partial x_j} + \sum_l \left(\Gamma_l - \Gamma_h\right) h_l \frac{\partial m_l}{\partial x_j} - \Gamma_h \frac{\partial}{\partial x_j}\left(\frac{u_i u_i}{2}\right)\right] \tag{1.13}$$

4. Species transport equations:

$$\frac{\partial \rho m_l}{\partial t} + \frac{\partial \rho u_j m_l}{\partial x_j} = \frac{\partial}{\partial x_j}\left(\Gamma_l \frac{\partial m_l}{\partial x_j}\right) + R_l \tag{1.14}$$

where $R_l$ is the production rate of specie $l$ caused by chemical reaction.

The above equations constitute the fundamental governing equations of chemical fluid mechanics. Obviously, these equations are exactly the same in formulation. They all contains four basic terms, which are an unsteady terms representing temporal variation, a convective term caused by macroscopic movement, a diffusive term related to the molecule movement, and source terms that do not belong to the above three terms. If $\varphi$ can represent general dependent variables ($u_i$,$h_0$,$m_l$), the fundamental equations can be written as a uniform expression of:

$$\frac{\partial \rho q}{\partial t} + \frac{\partial \rho u_j \varphi}{\partial x_j} = \frac{\partial}{\partial x_j}\left(\Gamma_\phi \frac{\partial \phi}{\partial x_j}\right) + S_\phi \tag{1.15}$$

where $\Gamma_\phi$ and $S_\varphi$ are the exchange coefficient and source terms depending on variable $\varphi$. They also can be referred to as transportation equations since the equations actually describe the diffusion and transportation processes of various physical variables. The variables following the transportation equations can be named as transportable variables. The transportation equations can be expressed in a uniform form. This fact reveals that the transportation process of variables has similar physical and mathematical characteristics. This can also benefit the numerical simulation as numerical methods and program coding can be expressed in a uniform form. All the equations can be solved using the corresponding $\Gamma_\phi$ and $S_\varphi$.

The above equations and gas mixture status equations can form closed equations. Theoretically, if the source term can be calculated using the knowledge from other subjects and boundary conditions are determined, the numerical solution of the combustion processes describing engines or other systems can be obtained. In fact, it would not be so easy since the flow and combustion in science and engineering are almost always turbulent process. Therefore, relevant modeling of turbulent flow and turbulent combustion is also necessary.

## 1.5 Outline of this Book

This book introduces numerical modeling of combustion processes in liquid rocket engines and its applications. The introduction of sub-processes such as atomization, liquid droplet evaporation, turbulent mixing, heat transfer, and combustion instability is first given as well as modeling and analysis methodology. Then, numerical tests and several applications are presented.

There are eight chapters in this book. The main content of each chapter is as follows:

- Chapter 1 is an introduction. The fundamental structures and working process of liquid rocket engines are first described, followed by the characteristics and history of numerical simulations of combustion process in liquid rocket engines. The governing equations of the chemical fluid mechanics are provided as well.
- Chapter 2 presents the atomization theory and research techniques, and atomization models for various types of injectors.
- Chapter 3 introduces the droplet evaporation combustion model. The droplet evaporation models under the normal and high pressure conditions are detailed. The response characteristics of a droplet in the pressure oscillation environment, multi-components droplet evaporation, and droplet group evaporation are discussed as well.
- Chapter 4 modelizes the turbulent flow and introduces the turbulence models for RANS simulation and sub-grid models for large-eddy simulation.

- Chapter 5 provides modeling of interaction of combustion and turbulence. The turbulent combustion model for RANS and sub-grid model for large-eddy simulation is given in this chapter.
- Chapter 6 describes models for heat transfer, heat convection, and heat radiation.
- Chapter 7 presents characteristics and theoretical models of combustion instability. Methods of controlling combustion instability and evaluation of these methods are detailed.
- Chapter 8 presents numerical models for atomization combustion in liquid rocket engines. Methods of grid generation and numerical methods of equations and models solution are provided as well as applications.

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# 2

# Physical Mechanism and Numerical Modeling of Liquid Propellant Atomization

In the combustor of a liquid rocket engine, the liquid propellant should first disintegrate into small droplets through the atomization process so that the fuel and oxidizer can evaporate quickly and mix well before combustion. Atomization plays a significant role in combustion stability and efficiency. It is important in engine design to investigate the atomization mechanism and atomization characteristics of injectors.

The atomization mechanism is essentially the same for all kinds of injectors used in liquid rocket engines. The liquid propellant first has to be expanded into a thin liquid film or jet [1]. When the jet speed is not high enough for the flow to develop into turbulence, perturbation waves on the liquid sheet or jet flow will grow rapidly under the action of the surface tension and aerodynamic force, resulting in the breakup of the liquid sheet/jet. The initial perturbations mainly arise from velocity fluctuations, nozzle vibration, and nozzle burr. When the jet develops into turbulent flow, turbulent eddies inside the jet determine the atomization process.

The main factors influencing the atomization performance of an injector:

1. internal flow characteristics determined by nozzle structures and operating conditions;
2. ambient gas parameters;
3. physical properties of liquid.

These factors should be included in the theoretical modeling of atomization. A large amount of work has been carried out on the breakup mechanism of liquid jet and liquid sheet and the resulting spray characteristics. However, there is still no one atomization model that can predict atomization characteristics for all kinds of injectors due to the complexity of the atomization process.

This chapter will describe the atomization mechanism of liquid propellant, evaluation parameters of atomization performance, and atomization model for nozzles that are in common

*Internal Combustion Processes of Liquid Rocket Engines: Modeling and Numerical Simulations*,
First Edition. Zhen-Guo Wang.

use in liquid rocket engines. Finally, the progress made in numerical simulations of atomization using interface tracking methods in recent years will be detailed.

## 2.1 Types and Functions of Injectors in a Liquid Rocket Engine

In a liquid rocket engine, propellant atomization is accomplished through the nozzles on the injecting panel under a certain injecting pressure. There are two advantages of atomization for the liquid fuel:

1. Beneficial for evaporation: Since evaporation is a surface process it occurs more quickly with a larger surface area for a certain amount of liquid. As the total surface area of drops with a certain amount of liquid mass is inversely proportional to their diameter, droplets with a smaller diameter will exhibit larger surface, which can accelerate the evaporation process. For example, while a spherical water drop of 1 kg only has a total surface area of 0.0483 $m^2$, the total surface area can increase to 60 $m^2$ after this water drop is atomized into droplets with a diameter of 50 μm. In a liquid rocket engine, the diameter of propellant droplets after atomization is in the range 25–500 μm, and thus the total surface of 1 $cm^3$ liquid propellant increases by tens of thousands of times through the atomization, which then accelerates the evaporation process.
2. Beneficial for mixing and combustion: while a kerosene droplet of 1 mm diameter needs at least 1 s to burn out in air, it can burn out in 0.025 s after being broken up into droplets of 50 μm diameter.

Depending on the pattern of injection holes on the face of an injector, injectors can be categorized into several types. The commonly-used injecting units include impinging injectors, coaxial straight-flow injectors, and coaxial swirl injectors. Impinging injectors can be classified into unlike impinging injectors and self-impinging injectors. The unlike doublet impinging injectors are often used in rocket engines with storable propellants, such as low-thrust control rocket engines, apogee rocket engines, and ascent engines of Apollo lunar modules. Self-impinging injectors are applied in rocket engines with spontaneously ignitable propellants. Coaxial injectors are commonly used in the $LOX/H_2$ cryogenic engines. Coaxial straight-flow injectors are commonly used in cryogenic propellant rocket engines in America, e.g., the main engines of space shuttles and the RL-10 engines of Atlas Centaur. In comparison with the coaxial straight-flow injectors, coaxial swirl injectors are less sensitive to unsteady combustion, and the injector number required in an engine with coaxial swirl injectors is less than that with coaxial straight-flow injectors. As part of the RL-10 series [2, 3], RL-10A-3, which used coaxial swirl injectors to improve the performance, was successfully developed. The American Space Transportation Main Engine (STME) also employed coaxial swirl injectors, and its stability was validated in experiments. In China, gas liquid coaxial swirl injectors have been employed in the development of cryogenic propellant rocket engines, with YF-75 as a representative example. A 50t $LOX/H_2$ rocket engine that can be used as the core stage of a CZ5 launcher has been successfully developed, and will undertake the mission of carrying a heavier payload together with 120t liquid oxygen/kerosene engines.

## 2.2 Atomization Mechanism of Liquid Propellant

In a liquid rocket engine, liquid propellants are fed into the combustion chamber in the form of a cylindrical jet or conical liquid sheet depending on the injector configuration. A significant part of the design of liquid rocket engines is to investigate the atomization mechanism of the cylindrical jet and conical liquid sheet. In the early research of atomization theory, the size of droplets resulting from fragmentation of the cylindrical jet and conical liquid sheet was calculated through theoretical models. However, the error of the calculated results is considerable in comparison with the experimental data due to the lack of influential factors in the model. As more of these factors are included in further developments, the theoretical model can produce better results. In this section, the size of liquid droplets dribbled from a pipe is analyzed, and the important role of the viscosity and surface tension in the formation of liquid droplets is also discussed. Then breakup models of liquid jet/sheet and droplet are introduced.

### *2.2.1 Formation of Static Liquid Droplet*

The formation of static liquid droplets is the typical form of atomization. Droplets dripping from a pipe is a classic example. When the gravitational pull on the liquid exceeds the surface tension acting on the pipe exit, the suspension state of the liquid is breached, and the liquid falls in the form of a droplet. The mass of the resulting droplet is determined by the gravity and the surface tension. The gravitational force on the droplet is equal to the surface tension acting on the pipe exit, resulting in the following relation:

$$m_{\mathrm{d}}g = \pi d\sigma \tag{2.1}$$

where:

d is the diameter of the pipe,
$m_{\mathrm{d}}$ is the mass of the droplet,
$g$ is the gravitational acceleration,
$\sigma$ is the surface tension coefficient.

The droplet diameter is:

$$D = \left(\frac{6d\sigma}{\rho_{\mathrm{l}}g}\right)^{1/3} \tag{2.2}$$

Here $D$ is the diameter of the formed droplet, and $\rho_{\mathrm{l}}$ is the density of the droplet.

For water, $\rho_{\mathrm{l}} = 1000$ kg m$^{-3}$, $\sigma = 0.07237$ N m$^{-1}$; and as for kerosene, $\rho_l = 800$ k m$^{-3}$, $\sigma = 0.023$ N m$^{-1}$.

When the pipe diameter ($d$) is 1 mm, the diameter of the generated water drop ($D$) is 3.6 mm and the kerosene droplet diameter ($D$) is 2.6 mm.

When $d = 10$ μm, the generated water and kerosene and drops are 765 and 560 μm, respectively, in diameter.