The Effect of Feedback in Thermal Spontaneous Combustion

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Abstract: In this paper, through the detailed analysis of the theory of thermal spontaneous combustion, the sufficient and necessary conditions for ignition in the cylinder of internal combustion engine are found out. Through the analysis of the three position relations between the reaction heat curve and the heat transfer curve, it can be concluded that the positive feedback is the necessary and sufficient condition for ignition. When the reaction heat curve intersects with the heat transfer curve, one intersection is the negative feedback attractor, and the other intersection is the critical ignition temperature. The analyses of these two intersections are not correct in many books. When the reaction heat curve is tangent to the heat transfer curve, the vessel wall temperature is the spontaneous combustion temperature. Feedback plays an important role in many working processes of internal combustion engine.

1. Introduction

Combustion in the cylinder of internal combustion engine is discontinuous; each cycle has a process of ignition. If the ignition process can not be completed smoothly, the internal combustion engine can not work, or cannot work in the stable state. The theory of thermal spontaneous combustion is one of the important theories in principles of internal-combustion engine and combustion science. It explains the process and conditions of ignition.

The theory of thermal spontaneous combustion was first put forward by Semonov. He pointed out that the necessary condition for spontaneous combustion and self explosion was, the heat released by slow chemical reaction could not pass through the wall of the container and disperse into the surrounding medium. When the temperature is not high, the reaction rate is slow. The heat released is less than the heat scattered into the surrounding medium, and the system keeps the balance. Without further heating, there will be no combustion or explosion. When we heat the gas to a critical temperature, that is to say, when the speed of reaction heat generation is exactly equal to, or a little faster than the speed of heat conduction, the substance will surely burn up, and this temperature is the ignition point.[1]

In order to simplify the calculation, Semonov uses the "zero dimension" model, which means to ignore the distribution of parameters like temperature and the reactant concentration in the container, and calculates all parameters in the whole system according to the average value. He assumed following conditions.

Firstly, the concentration and temperature of the mixture are the same everywhere in the container.

Secondly, in the reaction process, the reaction rate is the same everywhere in the container.

Thirdly, the temperature of the vessel wall T_0 and the temperature of the external environment remain unchanged during the reaction (the temperature difference determining the heat transfer intensity is the temperature difference between the wall and the mixture).

Fourthly, in the vicinity of ignition temperature, the change of the concentration of combustible gas mixture caused by reaction is ignored.[2]

Later studies gradually refined the description of the thermal spontaneous combustion process, and studied the specific ignition conditions according to different position relationships between the reaction heat curve and the heat transfer curve. But with the deepening of the research, problems emerge. Although researchers all regard the three relationships (intersection, tangency and

separation) of the two curves as the basis for determining the spontaneous combustion temperature, the ignition conditions are not pointed out accurately. Almost no one uses the concept and theory of feedback to analyze the process of thermal spontaneous combustion.

Feedback is the core concept of system theory. Negative feedback is the main method of automatic control; positive feedback is the main reason of explosion, internal combustion engine explosion, as well as many economic and social phenomena (such as stock market fluctuation, population explosion as well as the urban agglomeration effect). Positive feedback is also called as the Matthew effect or the benign (vicious) circle.[3] Both positive and negative feedback plays key roles in the ignition process. So, how to use the feedback theory to analyze the process of thermal spontaneous combustion?

2. The Feedback Relationship in Thermal Spontaneous Combustion Process

In the "zero dimension" model, if there is a vessel with a volume of V, which is full of uniform combustible gas mixture, and the combustible gas mixture in the vessel is reacting at a rate ω. Part of the heat released after the chemical reaction heats the gas mixture and raise the temperature of the reaction system, and the other part is transmitted to the surrounding environment through the vessel wall.

If we use q_1 to represent the heat released due to chemical reaction in unit time (J / s), then

$$q_1 = \omega q V \qquad (1)$$

In the formula, ω is the chemical reaction rate (mol/(m^3·s));
q is the molar heat effect of chemical reaction (J / mol);
V is the volume of container (m^3).
The chemical reaction rate ω is

$\omega = k_0 exp(-E / RT)c^n$

In the formula, $k_0 exp(-E / RT)$ is the reaction constant written according to the Arrhenius law;
k_0 is the reaction rate constant;
E is the activation energy (kJ / mol);
R is the gas constant;
T is the temperature of mixture(K);
c is the concentration of reactant (mol / m^3);
n is the reaction order.
If the reaction order n = 1, then
$\omega = k_0 exp(-E / RT)c$

Substituting the above formula into (1), then
$q_1 = qVk_0 exp(-E / RT)c$

Let $A = qVck_0$. According to the assumption of "zero dimension" model, A is a constant. Then the above formula can be written as

$$q_1 = Aexp(-E / RT) \qquad (2)$$

The heat transferred from the container to the surrounding environment in unit time q_2 is
$q_2 = aS(T - T_0)$

In the formula, a is the surface heat transfer coefficient $(W / (m^2 \cdot K))$;
S is the surface area of container (m^2);
T_0 is the vessel wall temperature (K).
The surface heat transfer coefficient a is related to the shape, size and material of the container. For a container with certain shape and size, aS is a constant. If $B = aS$, the formula can be written as

$$q_2 = B(T - T_0) \quad (3)$$

q_1 is an exponential curve, which is called the reaction heat curve; q_2 is a straight line, whose slope is aS, and is called the heat transfer curve. There are three kinds of relative position relations between the two curves, namely, intersection, tangency and separation. There are many factors that can affect the reaction heat and heat transfer, such as the change of cylinder pressure, different fuels and different combustion chamber structures, which will move, deflect or change the bending degree of the curves. But the reaction heat curve and heat transfer curve always have, and only have the above three relationships.

In most cases, the reaction heat curve and the heat transfer curve have two intersections, as shown in Figure 1. If the temperature of the combustible mixture is T_a, and the reaction heat rate of the mixture is equal to the heat transfer rate, namely $q_1=q_2$, the system temperature will remain unchanged at point A. When the temperature of the mixture deviates from T_a due to accidental reasons, assuming $T<T_a$ (i.e. moving to the left), because the reaction heat rate is greater than the heat transfer rate, namely $q_1>q_2$, the temperature will rise and the system will return to state A. On the contrary, when the working condition of the system accidentally deviates from point A, but it moves to the right because the reaction heat rate of the mixture is less than the heat transfer rate, that is, $q_1<q_2$, the temperature will drop and the working condition will return to state A.
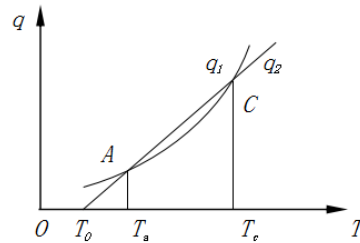

Fig.1 Reaction Heat Curve Intersect Heat Transfer Curve.

Therefore, no matter on the left or right side of point A, the system will eventually return to point A. Point A is the negative feedback equilibrium point, or the attractor. Unless there are external conditions to heat the mixture to T_c, the system will be always in the equilibrium state of condition A and can not be ignited.

For state C, the temperature of the mixture is T_c, and the reaction heat rate is equal to the heat transfer rate, that is, $q_1=q_2$. The temperature of the mixture remains unchanged and keeps the state of point C. When the working condition of the system accidentally deviates from point C and moves to the left, the reaction heat rate of the system is less than the heat transfer rate, that is, $q_1<q_2$. The temperature drops until the working condition returns to state A, and the system can not ignite at that time. That is, when $T<T_c$, the system is always a negative feedback system. When the working condition of the system accidentally deviates from point C and moves to the right, namely when $T>T_c$, the reaction heat rate of the system is greater than the heat transfer rate, $q_1>q_2$; the temperature will rise. The temperature rise will speed up the reaction heat rate, forming a positive feedback. The reaction rate in the system will accelerate and increase sharply, and then move farther and farther away from point C. It will eventually ignite or explode. T_c is the critical ignition temperature.

It can be seen that for the system, the ignition condition is that the mixture temperature $T>T_c$ and enters the positive feedback. If the mixture temperature can't reach T_c spontaneously, it needs some external conditions. For example, the ignition of the gasoline engine spark plug and the large compression ratio of the diesel engine can make the mixture temperature reach T_c. T_c is the forced ignition temperature [4] or the critical ignition temperature [2].

The tangency of the reaction heat curve and the heat transfer curve is shown in Figure 2. If the temperature of the mixture is T_b, and the reaction heat rate of the system is equal to the heat transfer rate, that is, $q_1=q_2$, the temperature will remain unchanged, and the state of point B will be maintained. When the working condition of the system accidentally deviates from point B and moves to the left, the reaction heat rate of the system is greater than the heat transfer rate, that is,

$q_1 > q_2$. The temperature will rise and the system will return to point B. At that time, the system is in the negative feedback state. However, once the working condition of the system slightly deviates from point B to the right, the system will enter into the state of positive feedback. The temperature will rise continuously, thus then lead to ignition. Therefore, when the reaction heat curve is tangent to the heat transfer curve, the tangent point B is the critical ignition point, and T_b is the critical ignition temperature. At this time, the vessel wall temperature T_0 is the spontaneous combustion temperature, or the critical environment temperature.
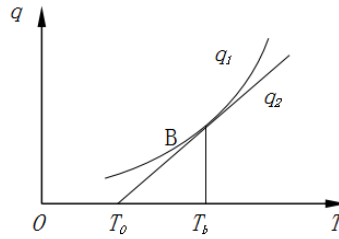

Fig.2 Tangency of Reaction Heat Curve and Heat Transfer Curve.

The case of no intersection between the reaction heat curve and the heat transfer curve is shown in Figure 3. Because the reaction heat rate is always greater than the heat transfer rate, that is, $q_1 > q_2$, the system will definitely catch fire. Because at that time, the system is always a positive feedback system.
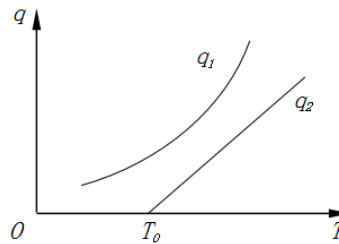

Fig.3 Reaction Heat Curve and Heat Transfer Curve Are Separate.

If the temperature of the vessel wall rises, the heat transfer curve will shift to the right; it may change from intersecting to be tangent with the reaction heat curve, and then separate from it, as shown in Figure 4. When they are separated, the ambient temperature is higher than the spontaneous combustion temperature, the system will catch fire. For example, in the operation of gasoline engine, when the cylinder wall temperature exceeds the spontaneous combustion temperature, the surface ignition phenomenon occurs. The combustion of gas does not depend on the spark plug ignition.
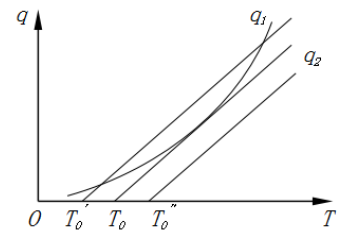

Fig.4 Transfer Heat Curve Moves.

If the system pressures are different, the reaction heat curve will change, and lead to the change of critical ignition temperature. The critical ignition temperature corresponding to each pressure value can be found, so a point can be obtained on the "critical ignition temperature - pressure" diagram. All these points can be linked to get a curve, as shown in Figure 5. The upper part of the curve is the ignition area and the lower part is the non ignition area. In the same way, we can get the "critical ambient temperature - pressure" diagram, the "critical combustion temperature - pressure" diagram, and the relationship diagram of other conditions.
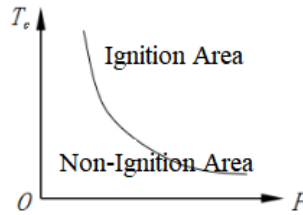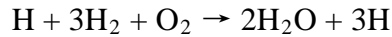
Fig.5 Relation of Critical Ignition Temperature and Press.

The chain chemical reaction of hydrogen combustion can be simply expressed as:

$$H + 3H_2 + O_2 \rightarrow 2H_2O + 3H$$

By this reaction, one hydrogen atom produces three hydrogen atoms. These three hydrogen atoms cause the next chain to produce more hydrogen atoms, which is called the chain reaction. This process is also a positive feedback. The larger cardinal number of H atom can cause more increments, which in turn leads to larger cardinal number of the next section. Finally the chain gets on fire. If the activation center is destroyed due to various reasons, resulting in too many chain breaks, the positive feedback cannot be formed. The chain can not be ignited. Therefore, positive feedback is also a necessary condition for chain ignition.

3. Problems in Existing Literature

In existing literature about combustion and engine theory, there are obvious problems in the theory of thermal spontaneous combustion. In various papers and books, although the characteristics of feedback are described, no one uses the concepts of positive feedback and negative feedback; no one mentions the inevitable relationship between feedback and ignition.

From the previous analysis, it can be seen that the system should be in a positive feedback state when it is able to ignite. When the heat reaction curve and the heat transfer curve intersect and $T > T_c$, when the two curves tangent and $T > T_b$, and when there is no intersection between the two lines, the system is in a positive feedback state. Therefore, in order to ignite, it is necessary for the system to be in a positive feedback state. To be in a negative feedback state is a sufficient condition for non-ignition.

In many documents, positive feedback state is called as the unstable state, while the negative feedback state is called the stable state. It is easy to lead to misunderstanding that the state of fire is not good and should be prevented, while the state of extinguishing is good. In fact, for the engine, we need such an unstable situation; the stability should be prevented from happening.

The two books of *Combustion of Internal Combustion Engine* (edited by Jiahua Chen and others) [5] and *Internal Combustion Engine Combustion Science* (edited by Xiangyi Wei) [6] also have the problems mentioned above. At the same time, they hold that it is impossible to ignite the system when the heat reaction curve intersects with the heat transfer curve, and believe that state *C* cannot be achieved. As mentioned before, state *C* can only be achieved under the condition of forced ignition. In case of forced ignition, the reaction heat curve and heat transfer curve are not changed, and the ignition conditions can be expressed by the intersection of the two lines. The theory of thermal spontaneous combustion can not only be used to analyze spontaneous combustion. It can also analyze forced combustion. Semonov's model includes forced combustion. Kefa Cen pointed out that the condition of forced ignition was $q_1=q_2$ [2], but he did not mention that the critical ignition temperature was the temperature T_c at point *C*. The compression ratio of diesel engine is high, and the temperature can reach T_c directly. At the same time, when the pressure increases, the heat reaction curve shifts upward and decreases T_c. The compression ratio of gasoline engine is low; in most cases, the local temperature reaches T_c because of the spark plug ignition. If none of these methods can bring the temperature to T_c, other measures are needed, such as adding hot water in winter to increase the ambient temperature, or using combustion improver to reduce T_c.

According to *Principles of Internal Combustion Engine* (edited by Deming Jiang), the

temperature can not automatically rise to point C at the intersection, so this point has no physical significance.[7] The two books *Motor Tractor Engine* (edited by Jing Dong and others) [8] and *Structure and Principle of Internal Combustion Engine* (edited by Yaozu Lu and others) [9] are relatively simple. They do not specifically cover above three situations. They simply introduce that the critical condition for ignition is the tangency of reaction heat reaction curve and heat transfer curve. Otherwise, if this condition can not be met, the system cannot be ignited.

According to the assumption of "zero dimension" model, the wall temperature T_0 and the temperature of the external environment remains unchanged in the reaction process. For the working process of the internal combustion engine, it remains the same in one working cycle, but it may change among different cycles. If the temperature of the vessel wall changes and the heat transfer curve moves, the two curves can change from intersection to tangent and separation, and the system can change from non ignition to ignition. In that case, the tangent point is meaningful. However, in the ignition or compression ignition process of one working cycle, the temperature of the container wall does not change and the heat transfer curve does not move. If the two curves do not change from intersecting to tangent, then the tangent point is meaningless; only the intersection C plays a role.

When analyzing the state of tangency between the heat reaction curve and the heat transfer curve, Deming Jiang called T_0 as the spontaneous combustion point, while Jiahua Chen thought that the temperature T_b at point B was the spontaneous combustion temperature. Chen believed that there was little difference between T_b and T_0, so T_0 was defined as the spontaneous combustion temperature [5] for convenience. That statement is not appropriate. The difference between T_b and T_0 cannot be ignored. T_0 is defined as the spontaneous combustion temperature because T_0 is more important than T_b. Because T_0 is relatively stable, but T_b is constantly changing. T_0 is easy to measure and control; T_b is almost impossible to measure and control. When the gasoline engine is working, the cylinder wall temperature T_0 can be controlled to avoid surface ignition. The importance of T_b lies in its theoretical significance, which should not be overstated.

4. Other Influences and Applications of Feedback in Internal Combustion Engines

Both positive and negative feedback plays important roles in many mechanisms and systems of the internal combustion engine. Here are some important feedback effects and applications.

Firstly, there is a float in the carburetor of the gasoline engine, which is used to keep the oil level of the float chamber stable. When the oil level rises, the float floats upward, and then the needle valve on the float is against the oil inlet. At that time, oil in the float chamber can only come out and cannot come in, so the oil level drops. When the oil level drops to a certain position, the buoyancy of the float decreases. The float drops and opens the needle valve; oil flows in from the oil inlet to raise the oil level of the float chamber. This process is the application of the negative feedback principle. It is also a negative feedback process to control the fuel injection quantity by sensors in the electronic controlled gasoline engine.

Secondly, the governor of the diesel engine is a mechanism which uses the negative feedback principle to adjust the rotate speed of the diesel engine. When the rotating speed increases, the centrifugal force of the flying hammer in the governor increases, so that the rotating radius increases. This change is transmitted to the oil supply rod through a set of levers, so as to reduce the amount of oil supply in each cycle and reduce the rotating speed. When the rotating speed decreases, the centrifugal force of the flying hammer decreases and the fuel supply increases.

Thirdly, if the diesel engine has no governor, it is easy to run out of control. When the rotating speed increases, the movement speed of the injector plunger increases; the effective stroke of the plunger also increases, so as to increase the quantity of fuel supply. The increase of fuel supply can increase the speed of diesel engine; the increase of diesel engine speed can increase the circulating fuel supply. The positive feedback is formed. This positive feedback can continuously increase the speed of the diesel engine; the engine loses control under that situation. Therefore, the diesel engine must be equipped with a governor, or use the electronic control to stabilize its speed.

Fourthly, knocking is the most important abnormal combustion phenomenon of the gasoline

engine. Serious knocking can not only beat the cylinder, reduce the power and cause smoke, but also increase the surface temperatures of the cooling system as well as the combustion chamber. The increasing temperature can lead to surface ignition easily, while the surface ignition can aggravate the knocking and form a positive feedback. The result of this positive feedback is to cause the violent knocking of the gasoline engine.

Apart from above examples, there are also many other effects and applications of feedback in internal combustion engines.

5. Conclusion

Most of the existing literature did not mention the concept of feedback when they talked about above contents. To study the working process of internal combustion engine and to implement effective control by applying feedback principle and system theory are effective ways to improve the performance of internal combustion engine.

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