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Simulation of a Stirling Engine with a Reversible Reaction $CO + 2H_2 \leftrightarrow CH_3OH$

Using a simple computer model, the properties of a Stirling engine are studied, where the working substance is a chemically reacting gas with a reversible reaction $CO + 2H_2 \leftrightarrow CH_3OH$. The model takes into account the relaxation time of hydrodynamic processes in the regenerator. In this case, the engine is considered to consist of three main parts: a heater, regenerator and a cooler, this is fundamental difference from the Langlois Justin model proposed in 2006. The pressure in the engine is 20 MPa, the working piston is free. The efficiency is compared for two cases: 1) a reversible chemical reaction occurs in the working gas and 2) the working gas is chemically inert with relatively high and low molar mass. The average power over the oscillation period is several hundred watts, but the maximum power can reach 2 kW. To increase the power of an engine with reversible chemical reaction, it is necessary to increase the volume of the cooler and reduce the volume of the heater. The modeling results are in good agreement with the previously obtained theoretical results of one of the authors (K. Sabdenov, 2023) based on the analysis of the Stirling cycle with reversible chemical reaction.

Keywords: Stirling cycle, free-piston Stirling engine, methanol, reversible chemical reaction, efficiency and power

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Introduction

The Stirling engine can produce electrical energy from any external heat source, including solar radiation. Therefore, it is considered as a promising means to solve the problem of energy shortages after the depletion of oil and natural gas reserves [1, 2].

In modern engines, the working gas is either chemically inert or can only react in one direction to form a combustion product. But the results of [3, 4] indicate a strong influence of the efficiency of various thermodynamic cycles due to the ongoing reversible chemical reaction in the working gas. If we compare it with a chemically inert gas, then such a reaction can lead to both a decrease and an increase in efficiency. In particular, high efficiency in the Stirling cycle can be obtained under the following conditions:

- at the compression stage, the working gas must have a higher molecular weight than at the expansion stage;
- the gas expansion coefficient must be sufficiently large;
- the maximum $T_{\min}$ (heater) and minimum $T_{\max}$ (cooler) temperatures should not differ significantly; this is due to the condition for the existence of a cycle.

The results of [3, 4] were obtained for ideal and equilibrium cycles, so they need to be confirmed either on real machines or on computer models. To do this, based on a computer model, the operation of a Stirling engine with a free working piston is studied. Its first mathematical model in the isothermal approximation was proposed in [5] and since then it has become the basis for many theoretical and experimental studies [6–11]. The isothermal approximation means assuming constant heater and cooler temperatures.

Cyclic changes in the dynamic parameters of the Stirling machine should be obtained as a result of solving the model equations expressing the laws of conservation of mass, momentum and energy. But in many theoretical studies, for example, in [7, 9–11], the coordinates of the working piston and displacer are specified in the form of a sinusoidal function. From the model [5] it is difficult to understand the physical mechanisms by which the machine operates and, most likely, it contains unjustified approximations and complications.

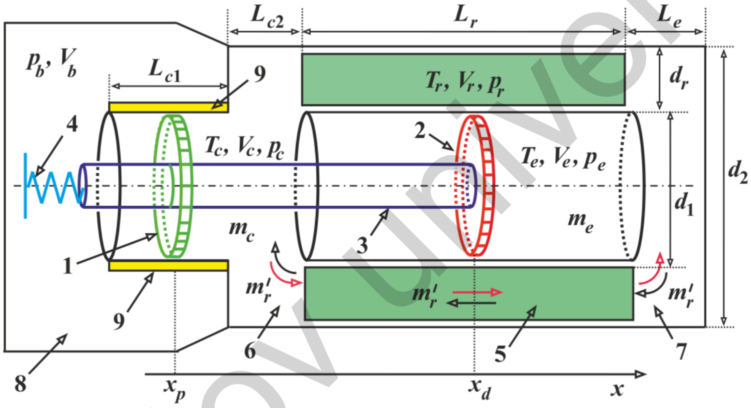
Experimental

This study has two objectives:

1) to build a simple model of a Stirling engine with a free piston, at the same time, the new model must take into account the most important physical properties of the engine;

2) using the constructed model of the Stirling engine, check the correctness of the results obtained from the thermodynamic analysis of a cycle with a reversible chemical reaction [3].

The general structure of the Stirling engine is described in detail in [5], therefore, below only the fundamental differences of the proposed device circuit are indicated. It is shown in Figure 1, here the cooler is combined with the volume (compression, 6) V_c, and the heater is combined with the volume (expansion, 7) V_e.



1 — working piston; *2* — displacer; *3* — displacer rod; *4* — displacer spring; *5* — regenerator; *6* — cooling area; *7* — heating area; *8* — buffer volume; *9* — linear electric generator

Figure 1. Simplified diagram of the structure of a Stirling engine with a free piston and the direction of the *x* coordinate

This means that the volumes V_c and V_e are essentially a cooler and a heater. Accordingly, they maintain constant temperatures T_c and T_e. They are taken as the minimum and maximum temperature in the car. The gas masses in each of the indicated volumes are equal to m_c and m_e.

Regenerator *5* continues to be present as an independent and important component of the machine, therefore it is characterized by its physical parameters.

Buffer space *8* with volume V_b and pressure p_b is borrowed from [5].

The working piston *1* moves freely along the rod *3* of the displacer *2*, the last two are rigidly connected to each other, and one of the ends of the rod is attached to the spring *4* with a stiffness coefficient k_d. The displacer can move freely inside the cylinder, surrounded by a cylindrical regenerator with length L_r and working space thickness d_r.

As a result of the movement of the working piston, the linear generator 9 generates an electric current, its reverse effect on the operation of the machine is taken into account by the damping coefficient D_p.

A Stirling engine cannot operate without a regenerator; the literature [12, 13] denies this, but points to the very low efficiency of a machine without a regenerator. Thus, although the regenerator is allocated a significant place, it is still not one of the main ones. In fact, in machines “without a regenerator” it is still present in a hidden and primitive form. Since the regenerator plays one of the key roles here, the processes in it need a detailed description. This mainly relates to gas flow.

The regenerator is represented by a narrow and long channel in the space between two coaxial cylinders with diameters d_1 and $d_2 = d_1 + 2d_r$. The average speed of one-dimensional gas motion in it with density ρ_r and in the direction of coordinate x will be denoted by u. Below is the momentum conservation equation for the elementary mass of the regenerator $\Delta m = \rho_r A_r \Delta x$, where the elementary volume in a section of length Δx and cross-sectional area A_r is equal to $A_r\Delta x$. This elementary volume is acted upon by two forces:

● the first of them F_p is associated with the change in pressure in space, $F_p = A_r(p(x + \Delta x) - p(x))$. If there is a local section on the path of gas movement at point $x = x_0$, then this section is characterized by the coefficient of hydraulic resistance K_r. Here the momentum of the flow changes, a force acts on it

$$F_p = \left(p(x+\Delta x) - p(x) + \frac{1}{2}\delta(x - x_0) K_r \rho_r |u| u \Delta x \right) A_r ,$$

where $\delta(x = x_0)$ is the Dirac delta function;

● the second force F_r arises as a result of the presence of friction inside the gas, and at the boundary of contact with the solid surface of the channel wall [14]. Friction forces lead to the appearance of tangential stress τ, and $F_{\text{fr}} = \tau \Pi \Delta x$.

From hydrodynamics [14], we accept the equality

$$\tau = \text{const} \cdot \zeta \rho_r |u| u ,$$

where ζ is the coefficient of hydrodynamic resistance; Π — channel perimeter, $\Pi = 2\pi(d_1 + d_r)$. Thus, we get

$$F_{\text{fr}} = \frac{1}{8} \cdot \zeta \rho_r \Pi |u| u \Delta x .$$

The 1/8 factor is explained below. Newton's second law can be written as

$$\Delta m \frac{du}{dt} = -A_r \frac{\partial p}{\partial x} \Delta x - \frac{1}{2} \delta(x - x_0) K_r \rho_r |u| u A_r \Delta x - F_{\text{fr}} .$$

Hence, after replacing the total time derivative in the sense of Lagrange with the derivative in the sense of Euler [14],

$$\frac{d}{dt} = \frac{\partial}{\partial t} + u \frac{\partial}{\partial x} ,$$

and also using the definition of mass Δm and in the limit $\Delta x \to 0$, the equation is obtained [15]

$$\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} = -\frac{1}{\rho_r} \frac{\partial p}{\partial x} - \frac{1}{8} \cdot \frac{\zeta \Pi}{A_r} |u| u - \frac{1}{2} \delta(x - x_0) K_r |u| u . \tag{1}$$

In typical Stirling machines, the thermal expansion of gas is small, the pressure also does not change much, and the compressibility of the gas is insignificant. Therefore, the derivative of density with time is small compared to convective transport. As a result, the mass flow $\rho_r u$ can only be a function of time. This means that the gas in the regenerator moves like a liquid and its speed is only a function of time. Therefore, instead of (1), we can consider the equation

$$\frac{du}{dt} = -\frac{1}{\rho_r} \frac{\partial p}{\partial x} - \frac{1}{8} \cdot \frac{\zeta \Pi}{A_r} |u| u - \frac{1}{2} \delta(x - x_0) K_r |u| u ,$$

where the partial derivative with respect to time is replaced by the total derivative, but in the Euler sense. Taking the gas velocity to be weakly dependent along the length of the regenerator, $\partial u / \partial x \approx 0$, by integrating over the length of the regenerator this equation is reduced to the form [15]

$$L_r \frac{du}{dt} = \frac{1}{\rho_r} \Delta p - \frac{1}{8} \zeta \frac{L_r \Pi}{A_r} |u| u - \frac{1}{2} K_r |u| u . \tag{2}$$

The pressure difference Δp is positive if the gas flows from left to right. Now let us explain the origin of the factor 1/8; in the stationary case and flow in a pipe, the well-known Darcy-Weisbach equation should be obtained [16]. In the case of an arbitrary pipe of length L_r and diameter D, the ratio $\Pi / A_r = 4/D$, and then it follows

$$\Delta p = \frac{1}{2}\zeta\rho_r \frac{L_r}{D}|u|u - \frac{1}{2}K_r\rho_r |u|u .$$

This is the Darcy-Weisbach equation for a pipe. For a regenerator (Fig. 1), the ratio of the perimeter to the flow area is $\Pi/A_r = 2/d_r$.

Equation (2) is relaxation, it takes into account the time required for the formation of gas velocity in the regenerator when pressure and friction change.

The model obtained above includes the equations of motion of the displacer, piston and gas in the regenerator. The coordinate of the displacer x_d with mass m_d is measured from the equilibrium position $x_{d,0}$, the initial coordinate of the piston x_p with mass m_p coincides with the coordinate reference point x.

The gas in the buffer volume compresses and expands under adiabatic conditions with index γ. External and initial pressure p_0.

The equations of motion of the displacer and piston have the form [5]

$$m_d \frac{d^2 x_d}{dt^2} + k_d(x_d - x_{d,0}) = p_b A_{rod} + p_c A_p - p_e A_d , \tag{3}$$

$$m_p \frac{d^2 x_p}{dt^2} + D_p \frac{dx_p}{dt} = (p_b - p_c)A_p . \tag{4}$$

The coefficient D_p characterizes the production of electrical energy by a linear generator. Equations (3) and (4) are supplemented with formulas for determining pressures:

$$p_b = p_0 \left(\frac{V_{b,0}}{V_b} \right)^{\gamma} , \tag{5}$$

$$p_c = \frac{R_{g,c} T_c}{V_c} m_c , \;\; p_e = \frac{R_{g,e} T_e}{V_e} m_e . \tag{6}$$

A change in the chemical composition of the gas leads to a change in the gas constant; the composition of the gas is different in the heater and cooler. Accordingly, two notations $R_{g,c}$ and $R_{g,e}$ are introduced for the gas constant.

The volumes contained here are found using the formulas

$$V_c = V_{c,0} + A_p(x_d - x_{d,0} - x_p), \tag{7}$$

$$V_e = V_{e,0} - A_d(x_d - x_{d,0}), \;\; V_b = V_{b,0} + A_{rod}(x_d - x_{d,0}) + A_p x_p .$$

Here $V_{c,0}$, $V_{e,0}$ are the initial volumes of the cooler and heater.

The gas masses in the displacer m_c and heater m_e are determined by solving the equations

$$\frac{dm_c}{dt} = -m'_r , \quad \frac{dm_e}{dt} = m'_r . \tag{8}$$

The gas mass flow rate m'_r in the regenerator is found from equation (2) and this issue is discussed below. The pressure p_r and temperature T_r in the regenerator are taken to be the average values in the heater and cooler:

$$p_r = \frac{p_e + p_c}{2} , \quad T_r = \frac{T_e + T_c}{2} . \tag{9}$$

Equalities (9) mean accepting a linear dependence on the x coordinate of changes in pressure and temperature in the regenerator. Linear dependencies are well fulfilled since the differences $p_c - p_e$ and $T_c - T_e$ are small values, and $d_r/L_r << 1$.

Then the gas density in the regenerator ρ_r is determined from the equation of state

$$\rho_r = \frac{p_e + p_c}{(T_e + T_c)R_g} . \tag{10}$$

Equation (10) is necessary to find the mass of gas in the regenerator m_r. Density ρ_r can be more accurately determined by calculating the average density using linear functions $p(x)$ and $T(x)$ and the gas equation of state for the regenerator [5]. But such averaging, which leads to a complex expression, does not provide noticeable advantages.

In Figure 1, between the regenerator and volumes V_c and V_e, there are local sections of gas flow rotation; they are included in the regenerator and are characterized by the coefficient K_r.

Equation (2) can also be written for mass flow $m'_r(t) = u(t)\rho_r A_r$. Using this definition and taking into account the constancy of density ρ_r, we write the equation for flow velocity,

$$\frac{dm'_r}{dt} = \frac{A_r}{L_r}\Delta p - \frac{1}{2}\frac{K_\Sigma \left|m'_r\right|}{m_r} m'_r, \tag{11}$$

$$K_\Sigma = K_r + \frac{L_r}{2d_r}\zeta, \quad m_r = \rho_r L_r A_r = \rho_r V_r, \quad V_r = L_r A_r. \tag{12}$$

According to Figure 1, the positive direction of gas movement corresponds to a positive sign of the pressure drop Δp, so it should be $\Delta p = p_c - p_e$.

Since the regenerator is a porous (mesh) structure made of thin metal wire [12, 13], then in the general case the porosity factor should be added to the determination of the gas volume V_r. Here it is assumed that the porosity is close to unity.

Let us denote by $m_{c,0}$ and $m_{e,0}$ the initial values of the gas masses in the cooler and heater, then from the sum of equations (8) and after integration the equality follows

$$m_c - m_{c,0} = -(m_e - m_{e,0}), \tag{13}$$

$$m_{c,0} = \frac{p_0 V_{c,0}}{R_{g,c} T_c}, \quad m_{e,0} = \frac{p_0 V_{e,0}}{R_{g,c} T_e}.$$

Chemical reactions of the first order take place in volumes V_c and V_e. In the first of them, the chemical transformation (reverse reaction) proceeds according to the scheme B → A at a rate k_c, and in the second (direct reaction) according to the scheme A → B at a rate k_e. At the same time, a mass of gas enters (or leaves) the indicated volumes at a speed m'_r; i.e. in each of them there can be two sources of substances of grade A and B. Each of them in an arbitrary volume has a mass m_{A} and m_{B}, their sum is always equal to the total mass of the gas in this volume. Substances A and B are characterized by relative mass concentrations g_{A} and g_{B}, and

$$g_{\mathrm{A}} + g_{\mathrm{B}} = 1. \tag{14}$$

For simplicity, the chemical transformation inside the regenerator is not taken into account. The simple connection (14) between concentrations allows us to subsequently use equations for only one of them, for example, g_{B}.

Since the gas mass in the cooler and heater is different, g_{B} will be determined in different ways. Therefore, below g_{B} is supplemented with indices indicating its value in V_c and V_e, i.e. $g_{\mathrm{B},c}$ and $g_{\mathrm{B},e}$. Using them, you can determine the gas constants $R_{g,c}$ and $R_{g,e}$ [17]:

$$R_{g,c} = R\left(\frac{g_{\mathrm{B},c}}{\mu_{\mathrm{B}}} + \frac{1-g_{\mathrm{B},c}}{\mu_{\mathrm{A}}}\right), \;\; R_{g,e} = R\left(\frac{g_{\mathrm{B},e}}{\mu_{\mathrm{B}}} + \frac{1-g_{\mathrm{B},e}}{\mu_{\mathrm{A}}}\right), \tag{15}$$

where R is the universal gas constant; μ_{A}, μ_{B} are the molar masses of substances A and B.

In the volume of the regenerator, the rates of forward and reverse chemical reactions are approximately equal. Since there is no change in the composition of the gas in the regenerator, when calculating the mass of gas in the regenerator m_r, the gas constant in it $R_{g,r}$ is determined by the conditions:

if $m'_r \geq 0$, then $R_{g,r} = R_{g,c}$; if $m'_r < 0$, then $R_{g,r} = R_{g,e}$.

Mass m_r is found from the equation of state

$$m_r = \frac{p_r V_r}{R_{g,r} T_r}.$$

The above data is sufficient to determine the parameters of the regenerator.

Consider the volume V_c and the <u>1st case</u> $m'_r > 0$, then the substance B will decrease due to convective entrainment from this volume and due to a chemical reaction. A simple first order reaction gives a conservation equation for the mass $m_{\mathrm{B},c}$,

$$\frac{dm_{\mathrm{B},c}}{dt} = -g_{\mathrm{B},c} m'_r - m_c k_c g_{\mathrm{B},c} \,. \tag{16}$$

According to the definition of relative mass concentration,

$$g_{\mathrm{B},c} = \frac{m_{\mathrm{B},c}}{m_c} \,.$$

Then, taking into account the first equality in (8), equation (16) can be written for $g_{\mathrm{B},\,c}$:

$$\frac{dg_{\mathrm{B},c}}{dt} = -k_c g_{\mathrm{B},c} \,. \tag{17}$$

In the <u>2nd case</u>, $m'_r < 0$ and the content of gas grade B changes both due to a chemical reaction and due to convective transfer from the heater. In volume V_e, the reaction A → B takes place. There, its concentration is designated $g_{\mathrm{B},\,e}$. The mass conservation equation will now take the form

$$\frac{dm_{\mathrm{B},c}}{dt} = -g_{\mathrm{B},e} m'_r - m_c k_c g_{\mathrm{B},c} \,.$$

After passing here to the concentration $g_{\mathrm{B},\,c}$, we obtain

$$\frac{dg_{\mathrm{B},c}}{dt} = \frac{g_{\mathrm{B},c} - g_{\mathrm{B},e}}{m_c} m'_r - k_c g_{\mathrm{B},c} \,. \tag{18}$$

In it, the reaction also has the first order, but now a substance of type B is formed. The derivation of equations for the concentration is carried out according to the same scheme as in the previous example. In the case $m'_r > 0$ for the mass $m_{\mathrm{B},\,e}$, the following equation is obtained:

$$\frac{dm_{\mathrm{B},e}}{dt} = g_{\mathrm{B},c} m'_r + m_e k_e (1 - g_{\mathrm{B},e}) \,.$$

To pass to the equation for the concentration $g_{\mathrm{B},\,e}$, we use the second equality in (8) and the definition $g_{\mathrm{B},\,e} = m_{\mathrm{B},\,e}/m_e$, as a result, we obtain

$$\frac{dg_{\mathrm{B},e}}{dt} = \frac{g_{\mathrm{B},c} - g_{\mathrm{B},e}}{m_e} m'_r + k_e (1 - g_{\mathrm{B},e}) \,. \tag{19}$$

In the case of $m'_r < 0$, the concentration $g_{\mathrm{B},\,e}$ is determined from the equation

$$\frac{dg_{\mathrm{B},e}}{dt} = k_e (1 - g_{\mathrm{B},e}) \,. \tag{20}$$

Results and Discussion

Equations (3), (4), (11) and (17)–(20) as well as one of the equations (8) are basic. To these are added auxiliary equalities (5)–(7), (9), (10), (12), (13) and (15).

The reversible reaction of methanol formation $CO + 2H_2 \leftrightarrow CH_3OH$ is considered [18, 19]. Substance A is a mixture of carbon monoxide and hydrogen with molar mass $\mu_A = 0.0107$ kg/mol; substance B is methanol with molar mass $\mu_B = 0.032$ kg/mol. At low temperature T_c, the decomposition reaction of methanol predominantly occurs according to the scheme B → A with the reaction constant k_c; at high temperature T_e, methanol is formed according to the scheme A → B with the reaction constant k_e.

The numerical solution of the equations was carried out by the Runge-Kutta method [20] with second order accuracy and with various time steps to verify the correctness of the results obtained. To obtain reliable results, it is enough to take the integration step equal to 10^{-4} s. Initial conditions:

$$t = 0: \quad x_p = 0,\ x_d = x_{d,0},\ \frac{dx_p}{dt} = 0,\ \frac{dx_d}{dt} = 1\,\mathrm{m/s};\ \ m'_r = 0,\ g_{b,c} = 0.15,\ g_{b,e} = 0.85 \,.$$

Electrical power P_{el} is always positive and equal to

$$P_{el} = D_p \left(\frac{dx_p}{dt} \right)^2 .$$

At the initial moment of time, the pressure in all volumes of the engine and outside was the same and equal to p_0; the mechanical system is in equilibrium. Then the total power of the engine P_m, or the rate of production of mechanical work, is equal to

$$P_m = \left| (p_c - p_e) \frac{dV_c}{dt} \right| + \left| (p_e - p_0) \frac{dV_e}{dt} \right| = \left| (p_c - p_e) A_p \left(\frac{dx_d}{dt} - \frac{dx_p}{dt} \right) \right| + \left| (p_e - p_0) A_d \frac{dx_d}{dt} \right| .$$

The necessity of the modulus sign is explained by the fact that useful work is performed both during expansion and compression of gas in volumes. Engine efficiency η_{el} was determined by the average power values P_{el} and P_m:

$$\eta_{el} = \frac{\langle P_{el} \rangle}{\langle P_m \rangle} .$$

The results in Figures 2–4 were obtained for the following input parameters:

- general and for buffer volume —

  $p_0 = 20$ MPa; $\gamma = 1.37$; $V_{b,0} = 2.0 \cdot 10^6\ \text{m}^3$ (the buffer volume is taken very large to exclude it);

- for displacer and working piston —

  $m_d = 3.0$, $m_p = 3.3$ kg; $k_d = 50\ \text{kg} \cdot \text{s}^{-2}$;

  $d_1 = 0.8$, $d_{rod} = 0.05$, $L_e = 0.3$ m; $D_p = 5500\ \text{kg} \cdot \text{s}^{-1}$;

- for heater and cooler —

  $T_c = 293$, $T_e = 673$ K; $V_{c,0} = 0.94$, $V_{e,0} = 0.54\ \text{m}^3$; $x_{d,0} = 1.6$ m;

  $k_c = 4.0 \cdot 10^{-2}$, $k_e = 4.2 \cdot 10^{-2}\ \text{s}^{-1}$; $L_{c1} = 1.0$, $L_{c2} = 0.5$ m;

- for regenerator —

  $L_r = 1.2$, $d_r = 0.1$ m; $A_r = 0.28\ \text{m}^2$; $K_r = 0.01$, $\zeta = 0.12$.

Work [21] gives a specific (per unit mass of copper catalyst) reaction constant for CO consumption of about $k_{\text{CO}} = 10^{-2}\ \text{mol}/(\text{kg}_{\text{cat}} \cdot \text{s})$. Here reaction constants of the order of 0.01…0.1 s^{-1} are used and in a different dimension. But a correlation can be established between these reaction constants: the gas volumes V_c and V_e are of the order of magnitude 10 mol. Then, taking 10 kg of catalyst (taking into account the high density of copper, such a mass of catalyst occupies a relatively small volume), we obtain $k_{\text{CO}} \sim 0.01\ \text{c}^{-1}$, which is comparable to the given value of k_e. The rate of the reverse reaction k_c is assumed to be approximately the same order of magnitude.

The oscillation of the displacer was established after approximately 70 s, its average position did not change (Fig. 2). But the average position of the piston shifts with a weak wave movement to the left along the x coordinate and by the time of 100 s it still has not reached its stationary point.

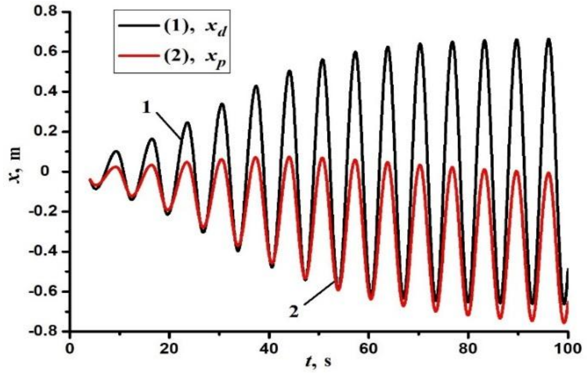


Figure 2. Coordinates of the displacer and piston depending on time

Power averaging (Fig. 3) was carried out over a time interval from 80 to 100 seconds, the results obtained were $\langle P_{el} \rangle = 355.3$, $\langle P_m \rangle = 906$ W; $\eta_{el} = 0.392$. The oscillation frequency is $\nu = 0.16$ Hz.

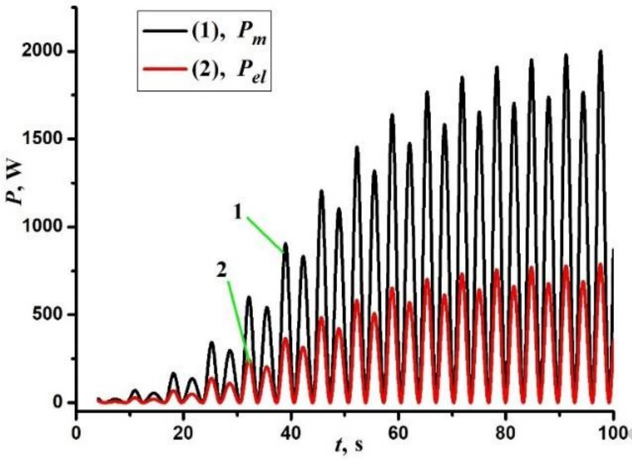


Figure 3. Dependence of powers P_m and P_{el} on time

The efficiency of an ideal Stirling cycle with a reversible chemical reaction η_{St} is characterized by a dimensionless parameter [3]

$$\alpha_{\mathrm{St}} = \frac{\mu_{\mathrm{B}}(\gamma_{\mathrm{B}} - 1)}{\mu_{\mathrm{A}}(\gamma_{\mathrm{A}} - 1)},$$

where γ_{A}, γ_{B} are the adiabatic exponent of substances A and B. The condition for exceeding η_{St} efficiency of the Carnot cycle with a chemically inert working gas η_0 is given by the inequality

$$\alpha_{\mathrm{St}} > \frac{T_{\max}}{T_{\min}}. \tag{21}$$

The γ_{A} exponent is easily determined, since detailed experimental data exist for the gases CO and H_2; from them it is easy to determine $\gamma_{\mathrm{A}} = 1.37$. The situation is more complicated with the adiabatic index of methanol γ_{B}; its physical properties change in a complex and ambiguous way depending on pressure and temperature [19], since it is located near the critical point. Therefore, in contrast to work [3], we use the formula from the theory of ideal gases [17]

$$\gamma_{\mathrm{B}} = \frac{i+2}{i},$$

where i is the number of degrees of freedom. From the structure of the methanol molecule it is easy to obtain the estimate $i = 10$, so we can take $\gamma_{\mathrm{B}} = 1.2$. This, together with $\gamma_{\mathrm{A}} = 1.37$, gives the value $\alpha_{\mathrm{St}} = 1.76$, and inequality (21) is not satisfied, since $T_{\max}/T_{\min} = 2.465$ ($T_{\max} = T_e$, $T_{\min} = T_c$). Accordingly, the efficiency according to the Carnot formula for a chemically inert working gas is equal to $\eta_0 = 1 - T_{\min}/T_{\max} = 0.565 > \eta_{el}$.

In [3] a formula was proposed for calculating the efficiency of an ideal Stirling cycle η_{St}; in the notation adopted here it has the form:

$$\eta_{\mathrm{St}} = 1 - \frac{T_{\min}}{T_{\max}} G(\omega), \tag{22}$$

$$G(\omega) = \frac{G_{0,1} + G_1}{G_{0,2} + G_1}, \quad G_1 = \left(1 + \frac{\mu_{\mathrm{B}} - \mu_{\mathrm{A}}}{\mu_{\mathrm{A}}} \frac{\omega}{\omega - 1}\right) \ln \omega,$$

$$G_{0,1} = \frac{1}{\gamma_{\mathrm{B}} - 1} \frac{T_{\max}}{T_{\min}} - \frac{\mu_{\mathrm{B}}}{\mu_{\mathrm{A}}(\gamma_{\mathrm{A}} - 1)}, \quad G_{0,2} = \frac{1}{\gamma_{\mathrm{B}} - 1} - \frac{\mu_{\mathrm{B}}}{\mu_{\mathrm{A}}(\gamma_{\mathrm{A}} - 1)} \frac{T_{\min}}{T_{\max}}.$$

Here there is a volume ratio ω on the upper (or lower) isotherm. This parameter ω depends on the engine design, so it can be found from the simulation results.

The cycle being implemented in the engine can be constructed in volume/pressure coordinates, since electrical energy is produced by the cooler, such a cycle is constructed in the variables $V_c/(p_c - p_0)$ in Figure 4 and bears little resemblance to the ideal cycle.

The lines are not closed because the piston has not yet reached the midpoint. But these data are sufficient to estimate the volume ratio $\omega = 1.28$ at points *2* and *1*. Then from equation (22) we find $\eta_{St} = 0.354$. This is less than the result obtained above $\eta_{el} = 0.392$ by approximately 10 %, and their difference may be introduced by the difference in the cycles in Figure 4 and ideal cycle, or, the approximate nature of equality (22). The fact is that when obtaining equation (22), a simple assumption was made of a linear dependence of the mass concentration of the product of a chemical reaction on the specific volume [3].

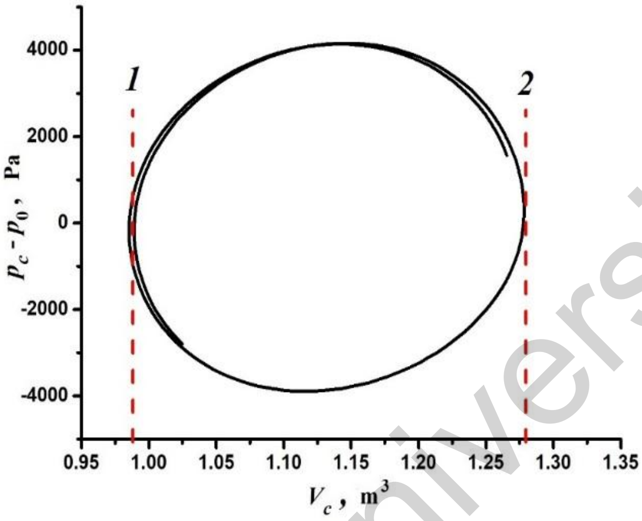


Figure 4. Image of the cycle in the Stirling engine in coordinates $V_c/(p_c - p_0)$,
the cycle is built for a time interval from 80 to 100 s

If we take the working gas to be a chemically inert substance with a molar mass of light gas $\mu_A = 0.0107$ kg/mol, then no displacement of the working piston is observed (Fig. 5).

However, all other input parameters remained unchanged. The engine reaches a steady state of operation in approximately 40 s. The frequency and amplitude of oscillations increased noticeably ($\nu = 0.17$ Hz), which explains the almost doubling of power: $\langle P_{el} \rangle = 684.6$, $\langle P_m \rangle = 1739$ W. There was also a very slight increase in electrical efficiency $\eta_{el} = 0.394$.

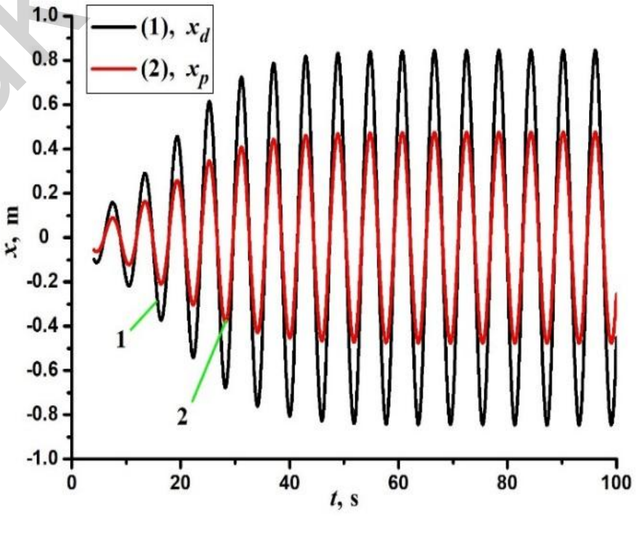


Figure 5. Changes in the coordinates of the displacer and piston over time
for a chemically inert working gas

For a chemically inert (relatively heavy) working gas with a molar mass $\mu_B = 0.032$ kg/mol, the working piston does not shift either. But the power and oscillation frequency are significantly reduced: $\langle P_{el} \rangle = 59.64$, $\langle P_m \rangle = 152.3$ W; $\nu = 0.10$ Hz. In addition, the time it takes for the engine to reach a steady state of operation increases; here this time is longer than the calculated time of 100 s.

From equation (22) it follows that efficiency increases with increasing expansion coefficient ω (at constant temperatures). To check this conclusion, the calculation was carried out with a change in the volume of the cooler by changing the length $L_{c,2}$. Below are the results for three options Table:

Table

$L_{c,2}$, m	ω	$\langle P_{el} \rangle$, W	$\langle P_m \rangle$, W	η_{el}	η_{St}
0.25	1.38	346	883	0.392	0.362
0.5	1.28	355	906	0.392	0.354
0.85	1.23	407	1037	0.392	0.350

No change in efficiency is observed, but engine power increases as the expansion coefficient decreases. Moreover, both total and electrical power increases proportionally, and a decrease in ω is achieved by increasing the volume of the cooler.

If you increase the volume of the heater while other parameters remain unchanged, then an increase in the volume of the heater leads to a decrease in power. For example, a calculation with a length $L_{c,2} = 0.5$, but with $L_e = 0.5$ m instead of the previous value $L_e = 0.3$ m gives $\langle P_{el} \rangle = 342$ and $\langle P_m \rangle = 873$ W.

Conclusions

In this study an isothermal model of a Stirling engine with a free piston and working gas, where a reversible chemical reaction occurs, is proposed. If we do not consider the presence of a chemical reaction, the new model differs from the previously proposed Langlois Justin model [5] by taking into account the relaxation time of hydrodynamic processes in the regenerator. Moreover, it consists of three main parts: heater, cooler and regenerator.

Based on the modeling results, the following conclusions were drawn:

- chemical transformation leads to a change in the molar mass of the gas mixture in the cooler and heater, as a result, during engine operation, the equilibrium position of the working piston shifts;
- such a shift occurs to the left if the molar mass of the gas is less than in the heater, if vice versa, then the piston moves to the right. Piston displacement does not occur in the case of gas with constant molar mass;
- the results of calculating the efficiency using the proposed model and the previously obtained formula for an ideal Stirling cycle with a reversible chemical reaction differ by approximately 10 %.

Conflict of interest statement

The authors declare that they have no conflict of interest in relation to this research, whether financial, personal, authorship or otherwise, that could affect the research and its results presented in this paper.

CRediT author statement

Sabdenov K.O.: Conceptualization, Methodology, Writing-Review & Editing; Smagulov, Zh.K.: Conceptualization, Methodology; Erzada, M.: Original Draft, Visualization, Software; Zhakatayev, T.A.: Original Draft, Software.

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Стирлинг қозғалтқышын қайтымды реакциямен $CO + 2H_2 \leftrightarrow CH_3OH$ модельдеу

Қарапайым компьютерлік модельдің көмегімен Стирлинг қозғалтқышының қасиеттері зерттелген, мұнда жұмыс заты $CO + 2H_2 \leftrightarrow CH_3OH$ қайтымды реакциясы бар химиялық әрекеттесетін газ қоспасы. Мұндай қозғалтқыш алғашқы рет қарастырылуда. Модель регенератордағы гидродинамикалық процестердің релаксация уақытын ескереді. Бұл жағдайда қозғалтқыш үш негізгі бөліктен тұрады: қыздырғыш, регенератор және салқындатқыш камералар, осы жаңа модель 2006 жылы ұсынылған Langlois Justin моделінен екінші түбегейлі айырмашылығымен сипатталады. Қозғалтқыштағы қысым 20 МПа, жұмыс поршені бос. Зерттеуде тиімділік екі жағдайда салыстырылады: 1) қайтымды химиялық реакция жұмыс газында жүреді және 2) жұмыс газы салыстырмалы түрде жоғары және төмен молярлық массасы бар химиялық инертті. Тербеліс кезеңіндегі орташа қуат бірнеше жүз ватт, бірақ максималды қуат 2 кВт-қа жетуі мүмкін. Қайтымды химиялық реакциясы бар қозғалтқыштың қуатын арттыру үшін салқындатқыштың көлемін ұлғайту және жылытқыштың көлемін азайту қажет. Модельдеу нәтижелері авторлардың бірінің бұрын алған теориялық нәтижелерімен жақсы сәйкес келеді (К. Сабденов, 2023) қайтымды химиялық реакциясы бар Стирлинг циклін талдауға негізделген.

Кілт сөздер: Стирлинг циклі, Стирлингтің бос поршенді қозғалтқышы, метанол, қайтымды химиялық реакция, ПӘК және қуат

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Моделирование двигателя Стирлинга с обратимой реакцией $CO + 2H_2 \leftrightarrow CH_3OH$

С помощью простой компьютерной модели впервые изучены свойства двигателя Стирлинга, где рабочим веществом является химически реагирующий газ с обратимой реакцией $CO + 2H_2 \leftrightarrow CH_3OH$. Модель учитывает время релаксации гидродинамических процессов в регенераторе. В данном случае двигатель считается состоящим из трех основных частей: нагревателя, регенератора и охладительной камеры. В этом состоит второе принципиальное отличие от модели Langlois Justin, предложенной в 2006 году. Давление в двигателе составляет 20 МПа, рабочий поршень свободен. Эффективность двигателя сравнивается для двух случаев: 1) в рабочем газе происходит обратимая химическая реакция и 2) рабочий газ химически инертен с относительно высокой и низкой молярной массой. Средняя мощность за период колебаний составляет несколько сотен ватт, но максимальная мощность может достигать 2 кВт. Чтобы увеличить мощность двигателя с обратимой химической реакцией, необходимо увеличить объем охладителя и уменьшить объем нагревателя. Результаты моделирования хорошо согласуются с ранее полученными теоретическими результатами одного из авторов (К. Сабденов, 2024), основанными на анализе цикла Стирлинга с обратимой химической реакцией.

Ключевые слова: цикл Стирлинга, свободнопоршневой двигатель Стирлинга, метанол, обратимая химическая реакция, КПД, мощность

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