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Calculation of Shock Wave Structures in Real Gas

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Abstract: The study considers the problem of calculating the shock-wave structures in calorically imperfect gas. An overview of calorically and thermally imperfect gas is provided. The dependence of adiabatic index on temperature for a diatomic gas is given. A comparison of this dependence with the linear approximation is performed. The concept of the effective adiabatic index at which the dynamic compatibility conditions have the same form as in the ideal gas is introduced. An algorithm for calculating the shock parameters using the effective adiabatic index is considered. The shock polars and shock reflections from the wall are calculated.

Key words: Adiabatic index, calorically imperfect gas, configuration, formation, mach number, pressure, shock, shock-wave structure, temperature

INTRODUCTION

The goal is to examine the calculation methodology of the shock-wave structures in calorically imperfect gas. The gas may be considered ideal in certain circumstances, i.e., non-viscous and non-conducting but must be imperfect. The gas is called imperfect when it does not satisfy the Mendeleev-Clapeyron equation of perfect gas state. For example, outside of shock wave and of boundary layer the influence of viscosity and heat conduction can be disregarded. But if the pressure or temperature is very high, the properties of the gas are substantially different from the properties of a perfect gas.

If the equation of gas dynamics includes the adiabatic index γ, then this is the equation of ideal, perfect gas. If the equation does not contain γ, it is suitable for any kind of gas. In a perfect gas γ is constant and is equal to:

$$\gamma = \frac{c_P}{c_V} \tag{1}$$

Where:

c_p = Heat capacity at constant pressure
c_v = Heat capacity at constant volume

Using the expression for the enthalpy (heat content is the energy that is available for conversion into heat at constant pressure), $H = c_pT$ as well as for the internal energy, $U = c_vT$, adiabatic index can be represented as the ratio of enthalpy to internal energy, $\gamma = H/U$. Specific heat c_p can be easily determined experimentally, c_v is usually calculated by the formula which follows from the equation of perfect gas state $c_v = c_pT\text{-}nR$ where n is number of substances in moles, R-universal gas constant, T-Temperature. In terms of the molecular-kinetic theory adiabatic index depends on the number of molecule's freedom degrees:

$$\gamma = \frac{i+2}{i} \tag{2}$$

It is assumed that the atoms in the molecule are linked tightly. In the one-atomic gas three are freedom degrees, corresponding to the three coordinates, then $\gamma = 5/3 \approx 1.67$. In diatomic gas two more freedom degrees are added which are associated with the molecule's rotation around two axes, $\gamma = 7/5 \approx 1.4$ in triatomic gas, one more rotational freedom degree is added, $\gamma = 8/6 \approx 1.33$. Adiabatic index for the following important gas mixtures are often emphasized:

- $\gamma = 1.1$: mixture of hydrocarbon fuel and air
- $\gamma = 1.2$: mixture of a hydrocarbon fuel with oxygen
- $\gamma = 1.25$: combustion product of hydrocarbon fuels

In the 21st century, the works on creation of the aircraft with jet engine of a new type, designed for high speed flight (M = 3.5-8) were began. Particular difficulties are posed by various non-stationary phenomena such as hysteresis, arising during the restructuration of shock-wave structure, low-frequency oscillations at the nasal (Zapryagaev and Kavun, 2007; 2008a, b) and at the bottom parts (Prodan, 2014; Bulat *et al.*, 2012; Bulat and

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Prodan, 2013) of aircraft, simulation of non-stationary shock-wave processes in engines associated with rotational and impulsive motion of shock waves. Since, the simulation of non-stationary turbulent flows with shock waves faces certain difficulties (Bulat and Bulat, 2013), the calculation is often carried out within the model of perfect gas. So, in research by Mitrofanov and Zhdan (2004), the cycle of the pulse-detonation engine's operation within the ideal gas model is numerically studied. By Adelman and Menees (1990) and Choi *et al.* (1998), it is shown that the known engine schemes with the formation of stationary detonation waves in air intakes are functional at Mach numbers of flight around 5-7. At the same time, it is known (Atafar *et al.*, 2013) that if there is a shock wave in the air ($T = 280°C$) with an intensity $J = 10$ (which corresponds to a normal shock in the stream with $M = 3$), then ignoring the dependence of y on the temperature leads to ≈8% error in calculation if gas temperature behind the shock. Therefore, constructing numerical methods it is relevant to account for deviations from the perfect gas model (Rydalevskaya *et al.*, 2014). In the monograph by Ben-Dor (2007), the analysis of the problem of oblique shock reflection from the wall with formation of regular two-wave configuration or three-wave Mach configuration is performed. During the analysis it is concluded that disregard of gas caloric imperfections is one of the main factor that causes the discrepancy of calculation results by the scheme of ideal perfect gas with the experiment. It is that task that was selected in present research as a demonstration.

MATERIALS AND METHODS

Mathematical model of a shock in the perfect gas

Two types of deviation from the ideal gas law: There are two types of deviations from the ideal gas law. Gas can accurately follow the equation of state for a perfect gas, but the specific heat capacities may not be permanent In this case, the gas called is thermally perfect but calorically imperfect. The gas can also have constant specific heats capacities but does not satisfy the equation of state perfect gas in such cases, the gas is called calorically perfect but thermally imperfect.

Specific heat capacity c_v increases at very high temperatures because vibrational freedom degrees of the molecules get exited. Thus, the adiabatic index will depend on the temperature and the gas will be calorically imperfect.

At normal temperature such phenomena do not occur. On the other hand when the gas density is high, so that, the average distance between molecules becomes small there is a considerable their interaction between them. Consequently, the equation of gas state may not coincide with the equation of state for perfect gas and thus, the gas would be calorically perfect and thermally imperfect.

Thus, it is necessary to distinguish two types of gas imperfections: caloric one, defined by excitation of different energy levels in the gas molecules and thermal one, defined by interaction between molecules. Adiabatic index can be calculated by experimentally determining the sonic speed in the gas environment:

$$a = \sqrt{\frac{\gamma R T}{\mu}} \tag{3}$$

where, μ = Molar mass. Let us, consider how the expression for sonic speed will look in a perfect gas. It is possible to divide the caloric and thermal imperfections of gas when examining it at zero pressure. Let's mark the internal energy at zero pressure as e_0, then e_0 is a function only of the temperature T. According to the second law of thermodynamics:

$$e(T, \upsilon_u) = \int_{\infty}^{\upsilon_u} \left[T\left(\frac{\partial p}{\partial T}\right)_{\upsilon_u} - p \right] d\upsilon_u + e_0(T) \tag{4}$$

Where:

υ_u = $1/\rho$ is specific volume of gas

ρ = Density

p = Pressure

For a perfect gas, the integral in Eq. 4 becomes zero and therefore, the internal energy and enthalpy does not depend on the pressure. The sonic speed can be calculated as follows:

$$a^2 = \left(\frac{dp}{d\upsilon}\right)_S = -\upsilon_u^2\left(\frac{dp}{d\upsilon_u}\right)_S = -\upsilon_u^2\left[\left(\frac{\partial p}{\partial T}\right)_{\upsilon_u}\left(\frac{dT}{d\upsilon_u}\right)_S + \left(\frac{\partial p}{\partial \upsilon_u}\right)_T\right] \tag{5}$$

From Eq. 4 differential equation for the derivative, included in Eq. 5 can be obtained:

$$\left(\frac{dT}{d\upsilon_u}\right)_S = -\frac{T\left(\frac{\partial p}{\partial T}\right)_{\upsilon_u}}{\frac{de_0}{dT}} \tag{6}$$

The index s in Eq. 4 and 5 means that the corresponding value is calculated for the isentropic process. Substituting Eq. 6 into Eq. 5, we obtain the final expression for the square of sonic speed:

$$a^2 = \upsilon_u \left[\frac{T\left(\frac{\partial p}{\partial T}\right)^2_{\upsilon_u}}{\frac{de_0}{dT}} - \left(\frac{\partial p}{\partial \upsilon_u}\right)_T \right] \qquad (7)$$

In the case of a perfect gas, the Eq. 7 is simplified to the Eq. 3 and sonic speed depends only on the temperature.

The dependence of heat capacity and of adiabatic index on the temperature: The gas imperfections are usually taken into account by adding various empirical constants and dependencies into the state equation of Mandeleev-Clapeyron. The most famous of these equations is the Vander Waals (Eq. 8):

$$P = \frac{\rho RT}{1-b\rho} - a\rho^2 \qquad (8)$$

in which the empirical constant a takes into account the mutual attraction of the molecules and constant b takes into account the fact that the molecules occupy certain non-zero volume. Berthelot (1899) upgraded this equation for very high temperatures (Tahmassebpour, 2016):

$$P = \frac{\rho RT}{1-b\rho} - \frac{a\rho^2}{T} \qquad (9)$$

Equation 9 allows obtaining an expression for the specific heat capacity at constant volume:

$$\left(\frac{\partial U}{\partial T}\right)_v = c_V \qquad (10)$$

At which the thermal and caloric effects of gas imperfections are separated. For this, let’s differentiate the equation by Joule-Thomson by temperature and obtain:

$$\frac{\partial}{\partial T}\left(\frac{\partial U}{\partial \upsilon}\right) = \frac{\partial}{\partial T}\left(T\left(\frac{\partial P}{\partial T}\right)_P - P\right) \qquad (11)$$

Changing the order of derivatives in Eq. 11, taking into account (Eq. 10), we can obtain the expression:

$$\left(\frac{\partial c_V}{\partial \upsilon}\right)_T = T\left(\frac{\partial^2 p}{\partial T^2}\right)_P \qquad (12)$$

Integrating it with regard to Eq. 9, we finally obtain:

$$c_V = \frac{2c\rho}{T^2} + c' \qquad (13)$$

The first member of Eq. 13 determines the dependence of the specific heat capacity on the density at high pressures, c' is the empirical constant that determines the strength of molecules interaction.

The second member of Eq. 13 is a constant that does not depend on the density but may depend on the temperature. From a physical point of view, the appearance of this constant indicates that the gas atoms in polyatomic molecules can oscillate and this will provide a further contribution to the internal energy level.

At normal temperatures, this effect can be ignored. For temperatures significantly different from the average, considering the atoms vibrations to be harmonic and gas to be diatomic, we can write (Eq. 14):

$$c' = c_{Vi}\left[1 + (\gamma_i - 1)\left(\frac{\theta}{T}\right)^2 \frac{e^{\theta/T}}{\left(1-e^{\theta/T}\right)^2}\right] \qquad (14)$$

Where:

C_{vi} = Specific heat capacity at constant pressure in ideal gas

θ = Energy constant equal 3056.4 K

To obtain heat capacity at constant pressure the expression, connecting two heats capacities is used:

$$c_p = c_V - T\frac{\left(\partial P/\partial T\right)^2_V}{\left(\partial P/\partial v\right)_T} \qquad (15)$$

Given that in an ideal gas $C_v = C_p - R$, we obtain:

$$c_p = c_{pi}\left[1 + \left(\frac{\gamma_i - 1}{\gamma_i}\right)\left\{\left(\frac{\theta}{T}\right)^2 \frac{e^{\theta/T}}{\left(1-e^{\theta/T}\right)^2} + \frac{2c\rho}{RT^2}\left[1 + \frac{\frac{2-b\rho}{1-b\rho} + \frac{c\rho}{2RT^2}}{\frac{1}{(1-b\rho)^2} - \frac{2c\rho}{RT^2}}\right]\right\}\right] \qquad (16)$$

Dividing Eq. 16 by Eq. 15 for the case of moderate pressure when the coefficients b and c can be considered values of second order, we obtain an expression for the dependence of the adiabat on the temperature:

$$\gamma(T) = 1 + \frac{\gamma_i - 1}{1 + (\gamma_i - 1)}\left[\left(\frac{\theta}{T}\right)^2 \frac{e^{\theta/T}}{\left(1-e^{\theta/T}\right)^2}\right] \qquad (17)$$

For each type of gases, Eq. 17 has a limit at $T\to\infty$. For instance with $\gamma i = 1.4$, γ (T) tends to 1.286.

Relations for calorically perfect gas at the shock: An obvious question arises whether it is possible to use the known dynamic compatibility conditions on the shock, derived from the conservation laws for perfect gas, to calculate the interference of shocks in an imperfect gas. The time required for the establishment of thermodynamic equilibrium in the gas behind the wave can be estimated by analyzing the speeds of chemical reactions. In those cases when the width of the relaxation layer is considered to be very small compared to the characteristic linear scale of the flow area, this layer together with the previous shock wave can be replaced by a single discontinuity.

In this model, the gas in front of the shock is in a "frozen" state and behind the shock in the equilibrium state. In the vicinity of discontinuity interference point, due to short residence time of the gas particles between incoming and outgoing breaks, the physical and chemical transformation behind the incoming breaks may be ignored and calculate the flow in this area may be performed according to the formulanffs of a perfect gas. Outside a close vicinity of interference point the flow is considered equilibrium and the parameters behind the shock are measured by the ratios:

$$\rho\upsilon_n = \widehat{\rho\upsilon_n},\ \rho\upsilon_n^2 - \widehat{\rho\upsilon_n^2} = \hat{p} - p,\ \upsilon_t = \hat{\upsilon}_t,\ i + \upsilon_n^2/2 = \hat{i} + \widehat{\upsilon_n^2}/2 \tag{18}$$

which connect the parameters at the shock front. In the Eq. 18 and further the "lid" indicates the parameters behind the shock. This allows us to write the energy equation (equation of shock adiabatic) in the form:

$$\hat{i} - i = \frac{1}{2}\frac{p}{\rho}(J-1)(1+E),\ E = \frac{\rho}{\hat{\rho}} \tag{19}$$

In a perfect gas the adiabatic index and molecular weight are constant, the values of p, ρ, T are connected by the state equation Mendeleev-Clapeyron and enthalpy (i) is directly proportional to temperature, i.e.:

$$i = \frac{\gamma}{\gamma-1}\frac{p}{\rho},\ \hat{i} = \frac{\gamma}{\gamma-1}\frac{\hat{P}}{\hat{\rho}} \tag{20}$$

Equation 19 taking into account the caloric Eq. 20, hence, follows Rankine-Hugoniot equation of shock adiabat:

$$E = (1+\varepsilon J)/(J+\varepsilon),\ \varepsilon = \frac{\gamma-1}{\gamma+1} \tag{21}$$

In the ideal, calorically imperfect gas the adiabatic index depends on the temperature but the caloric (Eq. 19) remains valid which allows to write it in quasi-perfect form:

$$i = \frac{\gamma_*}{\gamma_*-1}\frac{p}{\rho},\ \hat{i} = \frac{\hat{\gamma}_*}{\hat{\gamma}_*-1}\frac{\hat{P}}{\hat{\rho}} \tag{22}$$

In Eq. 22, the alternating adiabatic index is labeled, to distinguish it from the constant adiabatic index of ideal perfect gas. Then, the equation of the shock adiabat will take the form:

$$\frac{1+\hat{\varepsilon}_*}{\hat{\varepsilon}_*}JE - \frac{1+\varepsilon_*}{\varepsilon_*} = (J-1)(1+E) \tag{23}$$

It is possible to introduce the concept of effective adiabatic exponent γ_e, lying in the interval:

$$\gamma_e \subset [\gamma_*; \gamma_e] \tag{24}$$

The equation of the shock adiabat (Eq. 23) can be written in quasi-perfect form:

$$E = (1+\varepsilon_e J)/(J+\varepsilon_e) \tag{25}$$

Comparing Eq. 25 with Eq. 23, we obtain the expression for the effective adiabatic index γ_e:

$$\varepsilon_e/\varepsilon_* = 1 - (\varepsilon_* - \hat{\varepsilon}_*)(1 + \hat{\varepsilon}_*/J)/(\varepsilon_* J - \hat{\varepsilon}_*/J)\hat{\varepsilon}_* \tag{26}$$

Additionally, we can introduce the effective Mach number such that:

$$M_e^2 = \frac{\upsilon^2}{\gamma_e\frac{p}{\rho}},\ \hat{M}_e^2 = \frac{\hat{\upsilon}^2}{\gamma_e\frac{\hat{p}}{\hat{\rho}}} \tag{27}$$

Effective and local Mach number are connected by obvious relation:

$$\gamma M^2 = \gamma_e M_e^2 \tag{28}$$

Substituting γ_e and M_e in the dynamic compatibility conditions on the shock:

$$\hat{\upsilon}_n^2/\upsilon_n = 1 - \frac{P}{\rho\upsilon^2}(J-1)(1+E) \tag{29}$$

$$\sin^2\sigma = \frac{J-1}{1-E}\frac{P}{\rho\upsilon^2} \tag{30}$$

$$\mathrm{tg}\beta = \mathrm{tg}\sigma\left[1+\frac{E}{1-E}\left(1+\mathrm{tg}^2\sigma\right)\right]^{-1} \quad (31)$$

which follow from the conservation laws (Eq. 18), it is easy to verify that they have exactly the same form as those for a perfect gas. Therefore, the basic equations of oblique shock can be written in the form similar to the case of ideal perfect gas:

$$J = \left(1+\varepsilon_e\right)M_e^2\sin^2\sigma - \varepsilon_e \quad (32)$$

$$\hat{M}_e = \left[\frac{M_e^2-\left(1-E_e\right)\left(J+1\right)}{E_eJ}\right]^{1/2} \quad (33)$$

Thus, to calculate the shocks interference the well-known dynamic compatibility conditions (Eq. 29-31) and the basic relations for oblique shock (Eq. 32 and 33) obtained for the perfect gas can be used. Adiabatic index in this case is considered to be variable. In the case of calorically imperfect but thermally perfect gas, the adiabatic index is calculated using the relations (Eq. 17). If the gas is thermally imperfect as well the adiabatic index is determined from state equation for thermally imperfect gas.

RESULTS AND DISCUSSION

The influence of calorically imperfect gas on the shape of shock polar: Shock polar or shock isomach is the dependence of shock J intensity on the angle of flow rotation at the shock β, plotted for a given mach number before the shock. The problems of gas-dynamic discontinuities interference can often be conveniently solved by examining the intersection of shock polars, so, it is important to know how the shape of the polar will change with changing of temperature if the gas is calorically imperfect.

It shows the shock polar for Mach numbers M = 2.5 and M = 3.5, plotted at different temperatures before the shock. It is seen that the maximum shock intensity faintly depends on the temperature but the critical flow rotation angle of the shock is quite substantial.

Since, in the problem of studying the transition from regular to irregular reflection the key role is played by von Neumann separation criterion (when the shock polar touches the vertical axis), we can expect that the caloric imperfection of gas and as a result, the dependence of shock's limiting rotation angle on the temperature will significantly affect the moment of such transfer.

It shows the dependence of the limiting rotation angle at the shock at different temperatures and mach numbers before the shock. the black curve corresponds to T = 300 K, blue-T = 500 K, red-T = 1500 K.

It is seen that with increase of M the curves corresponding to T = 500 and 1500 K close together, tending towards asymptotical curve. Therefore, starting with M = 3 the asymptotic value of adiabatic index γ = 1.286 may be used for the flow behind the shock which eliminates the need to calculate it by iterations.

Regular and mach reflection of shock wave from the wall in calorically imperfect gas: It shows a diagram of the regular (left) and irregular (right) oblique shock reflection from a solid wall.

Below are the results of calculation reflected shock's intensity $\Lambda_2 = \ln J_2$ depending on the intensity of incident shock $\Lambda_1 = \ln J_1$. Two cases are considered: the irregular and regular reflection. Von Neumann criterion is used as a criterion for transition from regular to irregular reflection. This transition is accompanied by an abrupt change in the intensity of reflected shock. It is noticeable that the calorific gas imperfection affects both the moment of transition to irregular reflection and the value of abrupt change of reflected shock's intensity. The inset of shows the intensity of the main shock at the triple point T the intensity of mach stem. It can be seen that the highest difference is observed when the temperature before the first shock is within range of T = 300-1000 K, then it gradually decreases.

Shock intensity at different temperatures differs slightly but during the transition from regular to irregular reflection quite significantly.

From approximately 1000 K the offset of transition moment becomes less noticeable, therefore in this temperature range the asymptotic value of the adiabatic index can be used for calculation.

CONCLUSION

The influence of gas imperfections on the properties of the shock-wave structures has been examined. It has been shown that it is necessary to distinguish between caloric imperfection when the adiabatic index depends on temperature and thermal imperfection when high pressure causes the equation of ideal gas state to ceases to be satisfied. Formula for dynamic compatibility conditions on the shock derived for the perfect gas can also be used to calculate the calorically imperfect gas but taking into account the dependence of the adiabat on temperature. The above method of calculating the calorically perfect gas has demonstrated that with increasing temperature the value of the adiabatic index tends to its asymptotical which should be taken equal to the asymptotic value. Shock polars built for calorically perfect gas demonstrate the fact that the maximum intensity of the shock relatively weakly dependent on temperature. On the other hand, the effect of temperature on the value of limiting flow rotation angle is quite noticeable. This should be taken into account in the calculation of oblique shock reflection from the wall and of the interaction of colliding shocks. The most significantly the change of temperature affects the moment of transition from regular shock's reflection from wall to irregular one. Results were compared with numerical simulation performed on GPU with the use of advanced analysis methods (Gaidhane and Hote, 2016; Sivasuthan *et al.*, 2015; Rahmani *et al.*, 2011; Kunchur *et al.*, 2013, 2015; Raad *et al.*, 2016). It should be noted that even at a mach number of the original flow M = 3 and at normal temperature, calorific gas imperfection adds significant errors to the calculations and it should be mandatorily considered.

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