Computer Simulation of the Cylinder Process in a Compressor Based on the First Law of Thermodynamics

B. Karll
Danfoss A/S

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1. Introduction

Computer simulation is a general method of development and optimization, which is also used within the compressor industry.

Computer aided design (CAD) is used at several levels; rough but complex relations are simulated with advantage, thorough theoretical calculations as well.

The benefit of CAD depends on a reasonable choice of limits of the system described, i.e. at places where the boundary conditions are known and well defined; further that the level of the simulation is decided and maintained throughout the description.

Various problems require various limits, so it is advantageous to establish a library of subroutines from which a program pack for the actual job can be composed.

The following description of the cylinder process is an example illustrating such a subroutine. The description differs from the frequently used polytropic relation with an empirical exponent. The reason is that this relation does not describe the conditions during the open valve periods with reasonable accuracy.

Instead the cylinder process is treated theoretically. In this way the necessary empirical relations get a closer connection to the physical problems, which implies a better understanding and a wider validity.

2. Strategy

In the compressor simulation program the time \( t \) is the independent variable.

The cylinder process during a step in time, \( \Delta t \), is determined by the variation in two variables of state.

For practical reasons it has been decided to calculate the variation in specific volume \( \Delta v \) and temperature \( \Delta T \), but another choice would be equally justifiable.

The specific volume is determined by the fundamental variables, cylinder volume and the mass of gas in the cylinder.

The variation in temperature is given by the addition of heat and work to the gas.

An integration routine yields the value of the two variables at the end of the calculation step, and afterwards the equation of state and the other thermodynamic relations determine all other thermodynamic variables.

In appendix C the route diagram for the compressor simulation program is outlined.

3. The cylinder process

The change of the specific volume during a step in time is found from the cylinder volume \( V(a_1) \) and the mass of gas \( M \) in the cylinder before and after the interval:

\[ \Delta v = v_2 - v_1 \]

and

\[ \Delta v = \frac{V(a_1 + \Delta a)}{M_1 + \Delta M} - v_1 \]

Before the theoretical treatment of the variation in temperature, it is necessary to make some assumptions about the system.

The system is described as an enclosed mass of fluid to which heat and work are added. This description applies to the mass in the cylinder during periods with closed valves, and to the mass in a control space during a calculation step, with one of the valves open.

For this system the first law of thermodynamics applies

\[ u_2 - u_1 = Q + L \]

It is further assumed, that the mass of fluid is homogenous, so the equation can be related to unit of mass.

\[ u_2 - u_1 = q + L \]

This assumption simplifies the description extremely, and yields for example the state of the exhaust gas as a simple function of the state in the cylinder.

The assumption is reasonable due to the high level of turbulence in the cylinder, but when the piston is close to the top, the radial flow velocity can cause considerable discrepancy, which must be considered separately.

Assuming a reversible process the work is
given by
\[ \Delta L = -P \Delta v \] 3.5

The heat transferred to the system is calculated in another routine, by means of the temperature difference and the heat transfer coefficient on the limiting surfaces
\[ \Delta q = \sum k f A f (T_f - T) \Delta t / M \] 3.6

Consequently the variation in the internal energy is expressed in the cylinder process routine by
\[ \Delta u = \Delta q - P \Delta v \] 3.7

In appendix A the relation between \( \Delta u \) and \( \Delta T \) is derived; substituting this in (3.7) we arrive at the variation in temperature
\[ \Delta T = \frac{1}{c_v} \left( \Delta q - T \left( \frac{\partial P}{\partial T} \right)_v \Delta v \right) \] 3.8

c_v and \( \left( \frac{\partial P}{\partial T} \right)_v \) are calculated in a routine containing the thermodynamic relations. As an example they are derived in appendix B from a simple equation of state.

4. Suction and mixing

Suction and mixing during a time step is treated in two steps as illustrated by the figures 1 to 3.

Figure 1 indicates the situation before the interval. The cylinder volume \( A \), contains the mass \( M_1 \).

Figure 2 indicates the situation after the interval. The control space \( A \), contains the original mass, whereas the enclosed space \( B \), contains the mass \( \Delta M \), which has been sucked into the cylinder during the time interval.

Figure 3 indicates the situation after the mixing of the masses. Figure 2 and 3 represent the same moment, and the separation is introduced only to simplify the calculation.

Figure 2:
The state of the gas in the suction chamber is known, and the flow through the valve is assumed to stagnate in the cylinder with the original enthalpy. As the pressure in the cylinder is known, it is possible to calculate the state of the suction gas in space \( B \).

Here we introduce some simplifications; the pressure drop across the valve is small, and the refrigerant is almost a perfect gas, consequently the temperature and the internal energy in space \( B \) is approximately the same as in the suction chamber.

The mass and the state in space \( B \) is then
\[ M_B = \Delta M \]
\[ P_B = P_1 \]
\[ T_B = T_I \]
\[ u_B = u_I \] 4.1

From the equation of state the specific volume is found
\[ V_B = f(P_B, T_B) \] 4.2

The volume of space \( B \) is then
\[ V_B = \frac{M_B}{\rho} \] 4.3

The variation of state in space \( A \) during the time step, can now be determined. The variation in specific volume is given by equation (3.2) where \( \rho = \frac{M}{\rho} \).

The sum of internal energy in the cylinder is constant during the mixing process, so we have
\[ u_2 = \frac{M_A u_A + M_B u_B}{M_A + M_B} \] 4.4

and
\[ \Delta u = u_2 - u_1 \] 4.5

Finally the change of temperature is found by a transformation of equation (A7)
\[ \Delta T = \frac{1}{c_v} \left( \Delta u - (T \left( \frac{\partial P}{\partial T} \right)_v - P) \Delta v \right) \] 4.6

5. Conclusion

The equations governing the cylinder process in a compressor has been derived and can be programmed directly.

The theoretical treatment indicate the necessity of having a description of the heat transfer coefficient in the cylinder. This is not very well described today and should be emphasized in future research.

But even using a rough description of the
heat transfer, the cylinder process routine enables a better accordance with the physical reality than the polytropic relation, among others because it covers suction and discharge periods.

Appendix A

Temperature - internal energy relation:
The relation between increase in temperature and internal energy will be derived for a real gas, and expressed by the thermal variables of state.

The formal expression for a total differential is valid for the variables of state

\[ du = (\frac{\delta u}{\delta T})_v \, dT + (\frac{\delta u}{\delta v})_T \, dv \]

The specific heat at constant volume is defined by

\[ c_v = (\frac{\delta u}{\delta T})_v \]

From the second law in its differential form

\[ du = T \, ds - P \, dv \]

it follows that

\[ (\frac{\delta u}{\delta v})_T = T \, (\frac{\delta s}{\delta v})_T - P \]

Together with one of Maxwell's equations

\[ (\frac{\delta s}{\delta v})_T = (\frac{\delta p}{\delta T})_v \]

we have

\[ (\frac{\delta u}{\delta v})_T = T \, (\frac{\delta p}{\delta T})_v - P \]

Consequently, we have, from equation (A1), (A2) and (A6)

\[ du = c_v \, dT + (T \, (\frac{\delta p}{\delta T})_v - P) \, dv \]

Appendix B

Thermodynamic relations:
To show how \( \frac{\delta p}{\delta T} \) and \( c_v \) are related to the equation of state we use a simple equation as an example

\[ P = \frac{RT}{v-N_1+N_2/v} - \frac{N_4}{v^2} - \frac{N_5}{v^3} - \frac{N_6}{T \, v^3} \]

The partial derivative of the pressure with respect to the temperature with constant volume is

\[ \frac{\delta p}{\delta T} = -\frac{2 \, N_4}{T^3 \, v^2} + \frac{2 \, N_6}{T^3 \, v^3} \]

and hence

\[ T \, (\frac{\delta p}{\delta T})_v = P + \frac{N_4}{v^2} + \frac{2 \, N_4}{T \, v^2} + \frac{2 \, N_6}{T \, v^3} \]

The specific heat deviates from \( c_v \) at infinite volume

\[ c_v = c_{v\infty} + T \int_0^v \frac{\delta^2 p}{\delta T^2} \, dv \]

By differentiation of (B2)

\[ \frac{\delta^2 p}{\delta T^2} = -\frac{2 \, N_4}{T^3 \, v^2} + \frac{2 \, N_6}{T^3 \, v^3} \]

and the integration yields

\[ \int_0^v \frac{\delta^2 p}{\delta T^2} \, dv = \frac{2 \, N_4}{T^3 \, v} - \frac{N_6}{T^3 \, v^2} \]

Consequently we have from (B4)

\[ c_v = c_{v\infty} + \frac{2 \, N_4}{T^2 \, v} + \frac{N_6}{T^2 \, v^2} \]
Appendix C
Route diagram for the compressor simulation program: