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THERMODYNAMIC OPTIMIZATION OF SCREW COMPRESSORS

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Abstract: *A suitable procedure for optimization of the screw compressor shape, size, dimension and operating parameters is described here, which results in the most appropriate design for a given compressor application and fluid. It is based on a rack generation algorithm for rotor profile combined with a numerical model of the compressor fluid flow and thermodynamic processes. Some optimization issues of the rotor profile and compressor parts are discussed, using 5/6 screw compressor rotors to present the results. It is shown that the optimum rotor profile, compressor speed, oil flow rate and temperature may significantly differ when compressing different gases or vapors or if working at the oil-free or oil-flooded mode of operation.*

Key words: *thermodynamics, optimization, screw compressor, multivariable system.*

1. Introduction

Screw compressors are therefore efficient, compact, simple and reliable. They have largely replaced reciprocating machines in industrial applications and in refrigeration systems.

Screw compressors can be either single or multistage machines. Multistage are used for the compressor working with higher pressure ratios, while the single stages are used either for low pressure oil-free machines or moderate pressure oil-flooded compressors. A special challenge is imposed upon the multistage compressor optimization, because not only the compressor geometry parameters and operational conditions, but also the interstage pressures are optimized.

As other design processes, the design of screw compressors is an interactive feedback process where the performance of the compressor is compared with those specified in advance. Usually this is a manual process where the designer makes a prototype system which is tested and modified until it is satisfactory. With the help of a simulation model the prototyping can be reduced to a minimum. Recent advances in mathematical modeling and computer simulation can be used to form a powerful tool for the screw compressor process analysis and design optimization. Such models have evolved greatly during the past 10 years and, as they are better validated, their value as a design tool has increased. Their use has led to a steady evolution in screw rotor profiles and compressor shapes which should continue in future to lead to further improvements in machine performance.

A problem in optimization is a number of calculations which must be performed to identify and reach an optimum. Another problem is how to be certain that the optimum calculated is the global optimum.

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Among the optimization methods frequently used in engineering are steepest descent, Newton's method, Davidson–Fletcher–Powell's method, random search, grid search method, search along coordinate axes, Powell's method, Hooke–Reaves's method. A widely used method for optimization of functions with several optima is the genetic algorithm. It requires only a value of the target function and it can conveniently handle discontinuities, however this method is slow in converging to a solution. Alternatively a constrained simplex method, known as Box complex method can be conveniently used. Box complex method was therefore used here to find the local minima, which were input to an expanding compressor database. This finally served to estimate a global minimum. That database may be used later in conjunction with other results to accelerate the minimization. The constrained simplex method emerged form the evolutionary operation method which was introduced already in the 1950s by [1,2]. The basic idea is to replace the static operation of a process by a continuous and systematic scheme of slight perturbations in the control variables.

The effect of these perturbations is evaluated and the process is shifted in the direction of improvement. The basic simplex method was originally developed for evolutionary operation, but it was also suitable for the constrained simplex method. Its main advantage is that only a few starting trials are needed, and the simplex immediately moves away from unsuitable trial conditions.

There are several criteria for screw profile optimization which are valid irrespective of the machine type and duty. Thus, an efficient screw machine must admit the highest possible fluid flow rates for a given machine rotor size and speed. This implies that the fluid flow cross-sectional area must be as large as possible. In addition, the maximum delivery per unit size or weight of the machine must be accompanied by minimum power utilization for a compressor and maximum power output for an expander. This implies that the efficiency of the energy interchange between the fluid and the machine is a maximum. Accordingly unavoidable losses such as fluid leakage and energy losses must be kept to a minimum. Therefore, increased leakage may be more than compensated by greater bulk fluid flow rates. However, specification of the required compressor delivery rate requires simultaneous optimization of the rotor size and speed to minimize the compressor weight while maximizing its efficiency. Finally, for oil-flooded compressors, the oil injection flow rate, inlet temperature and position needs to be optimized. It follows that a multivariable minimization procedure is needed for screw compressor design with the optimum function criterion comprising a weighted balance between compressor size and efficiency or specific power.

2. Minimization Method Used in Screw Compressor Optimization

The power and capacity of contemporary computers is only just sufficient to enable a full multivariable optimization of both the rotor profile and the whole compressor design to be performed simultaneously in one pass.

The optimization of a screw compressor design is generically described as a multivariable constrained optimization problem. The task is to maximize a target function $f(x_1, x_2, ..., x_n)$, subjected simultaneously to the effects of the explicit and implicit constraints and limits:

$$g_i \le x_i \le h_i,\ i = 1, n$$

and

$$g_i \le y_i \le h_i,\ i = 1, n+1, m$$

respectively, where the implicit variables y_{n+1}, y_m are dependent functions of x_i. The constraints g_i and h_i are either constants or functions of the variables x_i.

When attempting to optimize a compressor design a criterion for a favorable result must be decided, for instance the minimum power consumption, or operation cost. However, the power consumption is coupled to other requirements which should be satisfied, for example a low compressor price, or investment cost. The problem becomes obvious if the requirement for low power consumption conflicts with the requirement of low compressor price. For a designer, the balance is often completed with sound judgment. For an optimization program the balance must be expressed in numerical values. This is normally done with weights on the different parts of the target function.

An important issue for real-world optimization problems is constraints. In the general case, there are two types of constraints, explicit or implicit. The explicit ones are limitations in the range of optimized parameters, for example available component sizes. These two different constraints can, in theory, be handled more or less in the same way. In practice, however, they are handled differently.

The implicit constraints are often more difficult to manage than explicit constraints. The most convenient and most common way is to use penalty functions and thus incorporate the constraints in the objective function. Another way is to tell the optimization algorithm when the evaluated point is invalid and generate a new point according to some predetermined rule. Generally, it can be said that constraints, especially implicit constraints, make the optimization problem harder to solve, since it reduces the solution space.

In the early 1960s, a method called the simplex method emerged as an empirical method for optimization, this should not be confused with the simplex method for linear programming. The simplex method was later extended by [3] to handle constrained problems. This constrained simplex method was appropriately called the complex method, from constrained simplex. Since then, several versions have been used. Here, the basic working idea is outlined for the complex method used. If the nonlinear problem is to be solved, it is necessary to use k points in a simplex, where $k = 2n$. These starting points are randomly generated so that both the implicit and explicit conditions in are satisfied. Let the points x^h and x^g be defined by

$$f\left(x^h\right) = \max f\left(x^1\right), f\left(x^2\right), \ldots, f\left(x^k\right)$$
$$f\left(x^g\right) = \min f\left(x^1\right), f\left(x^2\right), \ldots, f\left(x^k\right) \qquad (1)$$

3. Calculation of Thermodynamic Processes in Screw Compressor Optimization.

The algorithm of the thermodynamic and flow processes used in optimization calculations is based on a mathematical model comprising a set of equations which describe the physics of all the processes within the screw compressor. The mathematical model gives an instantaneous operating volume, which changes with rotation angle or time, together with the differential equations of conservation of mass and energy flow through it, and a number of algebraic equations defining phenomena associated with the flow. These are applied to each process that the fluid is subjected to within the machine; namely, suction, compression and discharge. The set of differential equations thus derived cannot be solved analytically in closed form. In the past, various simplifications have been made to the equations in order to expedite their numerical solution. The present model is more comprehensive and it is possible to observe the consequences of neglecting some of the terms in the equations and to determine the validity of such assumptions. This provision gives more generality to the model and makes it suitable for optimization applications. A feature of the model is the use the energy equation in the form which results in internal energy rather than enthalpy as the derived variable. This was found to be computationally more convenient, especially when evaluating the properties of real fluids because their temperature and pressure calculation is not explicit. However, since the internal energy can be expressed as a function of the temperature and specific volume only, pressure can be calculated subsequently directly. All the remaining thermodynamic and fluid properties within the machine cycle are derived from the internal energy and the volume and the computation is carried out through several cycles until the solution converges. The working fluid can be any gas or liquid–gas mixture, i.e. any ideal or real gas or liquid–gas mixture of known properties. The model accounts for heat transfer between the gas and compressor and for leakage through the clearances in any stage of the process. The model works independently of the specification of compressor geometry. Liquid can be injected during any of the compressor process stages. The model also takes in consideration the gas solubility in the injected fluid. The thermodynamic equations of state and change of state of the fluid and the constitutive relationships are included in the model. The following forms of the conservation equations have been employed in the model. The conservation of internal energy is:

$$\omega\left(\frac{dU}{d\theta}\right) = \dot{m}_{in}h_{in} - \dot{m}_{out}h_{out} + \dot{Q} - \omega p\frac{dV}{d\theta} \tag{2}$$

$$\dot{m}_{in}h_{in} = \dot{m}_{suc}h_{suc} + \dot{m}_{l,g}h_{l,g} + \dot{m}_{oil}h_{oil} \tag{3}$$

$$\dot{m}_{out}h_{out} = \dot{m}_{dis}h_{dis} + \dot{m}_{l,l}h_{l,l} \tag{4}$$

where h and x are angle and angular speed of rotation of the male rotor respectively, $h = h(\theta)$ is specific enthalpy, $\dot{m} = \dot{m}(\theta)$ is mass flow rate going in or out, $p = p(\theta)$ is fluid pressure in the working chamber control volume, $\dot{Q} = \dot{Q}(\theta)$, heat transfer between the fluid and the compressor surrounding, $\dot{V} = \dot{V}(\theta)$ local volume of the compressor working chamber. In the above equation the index in denotes inflow and the index out the fluid outflow. Oil and leakage are denoted by indices oil and l.

The mass continuity equation is:

$$\omega\frac{dm}{d\theta} = \dot{m}_{in} - \dot{m}_{out} \tag{5}$$

The instantaneous density $\rho = \rho(\theta)$ is obtained from the instantaneous mass m trapped in the control volume and the size of the corresponding instantaneous volume V as $\rho = m/V$.

The suction and discharge port flows are defined by velocity through them and their cross section area

$$\dot{m}_{in} = w_{in}\rho_{in}A_{in}, \qquad (6)$$
$$\dot{m}_{out} = w_{out}\rho_{out}A_{out}$$

The cross-section area A is obtained from the compressor geometry and it was considered as a periodical function of the angle of rotation θ.

Leakage in a screw machine forms a substantial part of the total flow rate and plays an important role because it affects the delivered mass flow rate and compressor work and hence both the compressor volumetric and adiabatic efficiencies.

$$\dot{m}_l = w_l\rho_l A_l = \sqrt{\frac{p_2^2 - p_1^2}{a^2\left(\varsigma + 2\ln\frac{p_2}{p_1}\right)}} \qquad (7)$$

where a is the speed of sound, ς is a compound resistance coefficient and indices l, 1 and 2 represent leakage, upstream and downstream conditions.

Injection of oil or other liquids for lubrication, cooling or sealing purposes, modifies the thermodynamic process in a screw compressor substantially. Special effects, such as gas or its condensate mixing and dissolving in or flashing out of the injected fluid must be accounted for separately if they are expected to affect the process. In addition to lubrication, the major purpose for injecting oil into a compressor is to seal the gaps and cool the gas. Flow of the injected oil, oil inlet temperature and injection position are additional optimization variables if the oil-flooded compressors are in question. Heat transfer between oil and gas is modeled as a first order dynamic system.

$$\frac{dT_{oil}}{d\theta} = \frac{h_{oil}A_{oil}\left(T - T_{oil}\right)}{\omega\dot{m}_{oil}c_{oil}}$$
$$T_{oil} = \frac{T - kT_{oil,p}}{1+k} \qquad (8)$$
$$k = \frac{\omega_{oil}\dot{m}_{oil}c_{oil}}{h_{oil}A_{oil}\Delta\theta}$$

k is, therefore, a time constant and h and A are the heat transfer coefficient between oil and gas and effective area surface based on the mean Sauter diameter d of the oil droplet. c is specific heat. $\Delta\theta$ is a time step and index p denotes previous.

The solution of the equation set in the form of internal energy U and mass m is performed numerically by means of the Runge–Kutta fourth order method, with appropriate initial and boundary conditions. As the initial conditions were arbitrary selected, the convergence of the solution is achieved after the difference between two consecutive compressor cycles becomes sufficiently small.

Once solved, internal energy $U(\theta)$ and mass in the compressor working chamber $m(\theta)$ serve to calculate the fluid pressure and temperature.

Since $U(\theta) = (mu) + (mu)_{oil}$, specific internal energy is:

$$u = \frac{U - (mcT)_{oil}}{m} \qquad (9)$$

As volume $V(\theta)$ is known, a specific volume is calculated as $v = V/m$. Therefore, temperature T and pressure p for ideal gas can be calculated as:

$$T = (\gamma - 1)\frac{u}{R}, \quad p = \frac{RT}{v} \qquad (10)$$

where R and γ are gas constant and isentropic exponent respectively. In the case of a real gas, $u = f_1(T, v)$ and $p = f_2(T, v)$ are known functions and should be solved to obtain the fluid temperature and pressure T and p. This task is simplified because internal energy u is not a function of pressure, therefore, f_1 and f_2 can be solved in a sequence. In the case of a wet vapor because of the fluid phase change either through evaporation or condensation, the saturation temperature and pressure determine each other between themselves and also the liquid and vapor internal energy and volume, u and v. Indices f and g denote liquid and gas phases. Therefore, vapor quality x can be calculated by successive approximations of u. Variables T or p and v can be obtained from:

$$u = (1-x)u_f + xu_g,\quad v = (1-x)v_f + xv_g \tag{11}$$

Numerical solution of the mathematical model of the physical process in the compressor provides a basis for a more exact computation of all desired integral characteristics with a satisfactory degree of accuracy. The most important of these properties are the compressor mass flow rate $\dot{m}$ [kg/s], the indicated work W_{ind} [kJ] and power P_{ind} [kW], specific indicated power P_s [kJ/kg], volumetric efficiency η_v, adiabatic efficiency η_i and isothermal efficiency η_t. Z_1 and n are the number of lobes in the main rotor and main rotor rotational speed. F_1 , F_2 and L are the main and gate rotor cross section and length. Index s means theoretical and indices t and a denote isothermal and adiabatic. Isothermal W_t and adiabatic work W_a and are given here for ideal gas.

$$m = m_{in} - m_{out},\quad W_{ind} = \int_{cycle} Vdp \tag{12}$$

$$\dot{m} = mz_l\, n/60,\quad P_{ind} = \frac{W_{ind} z_l n}{60} \tag{13}$$

$$\dot{m}_s = \frac{(F_{1_n} + F_{2_n})Lnz_1\rho}{60} \tag{14}$$

$$W_1 = RT_1 \ln\frac{p_2}{p_1},\quad W_2 = \frac{\gamma}{\gamma-1}R(T_2 - T_1) \tag{15}$$

A full and detailed description of the presented model of the compressor thermodynamics is given in [7].

$$\eta_v = \frac{\dot{m}}{\dot{m}_s},\ \eta_t = \frac{W_t}{W_{ind}},\quad \eta_i = \frac{W_a}{W_{ind}},\ P_s = \frac{P_{ind}}{\dot{V}} \tag{16}$$

Compressor speed is used as the compressor operating variable and oil flow, temperature and oil injection position are oil optimization parameters. Each of these rotor variables has its own influence upon the compressor process which is qualitatively explained in the following qualitative diagrams, Figs. 1 and 2.

Compressor shaft speed increases dynamic losses and decreases relative leakages. These two opposing effects cause that therefore, an optimum value of the shaft speed exists which gives the best compressor performance.

In oil-flooded compressors oil is used to lubricate the rotors, seal the leakage gaps and cool the gas compressed. Therefore its influence upon the compressor process is complex.

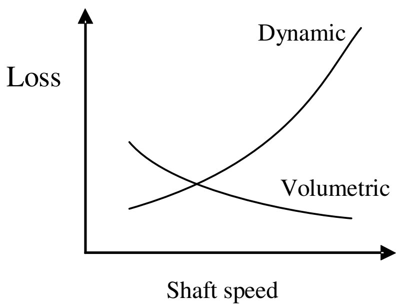

Fig. 1. *Influence of the compressor shaft speed upon the compressor volumetric and dynamic losses*

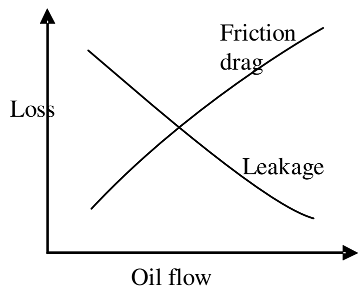

Fig. 2. *Influence of the injected oil flow upon leakage and friction drag losses*

More oil improves the compressor volumetric efficiency and also improves cooling, however, it increase the friction drag between the rotors themselves and between the rotors and housing. Obviously an oil flow rate exists which will produce the best compressor performance. Each of the described geometry and operating parameters influences the compressor process on its own way and only a simultaneous minimization, which takes into consideration all the influences together will produce the best overall compressor performance. Therefore only a multivariable optimization finds its full sense in the evaluation of the best compressor performance.

4. Conclusions

A full multivariable optimization of screw compressor geometry and operating conditions has been performed to establish the most efficient compressor design for any given duty. This has been achieved with a computer package for modeling compressor processes, developed by the authors, which provides the general specification of the lobe segments in terms of several key parameters and which can generate various lobe shapes and simultaneously calculates compressor thermodynamics.

Computation of the instantaneous cross-sectional area and working volume could thereby be calculated repetitively in terms of the rotation angle. A mathematical model of the thermodynamic and fluid flow process is contained in the package, as well as models of associated processes encountered in real machines, such as variable fluid leakages, oil flooding or other fluid injection, heat losses to the surroundings, friction losses and other effects. All these are expressed in differential form in terms of an increment of the rotation angle. Numerical solution of these equations enables the screw compressor flow, power and specific power and compressor efficiencies to be calculated.

References

1. Box, M.J.: *A new method of constrained optimization and a comparison with other methods*. In: Computer Journal 8 (1965) 42–52.
2. Fleming, J.S., Tang, Y., Xing, Z.W., Cook, G.: *The use of superfeed in a refrigeration plant with a twin screw compressor: an optimization technique for plant design*. In: IIR XIX Congress, The Hague, The Netherlands, 1995.

3. Hanjalic, K., Stosic, N.: *Development and optimization of screw machines with a simulation model*, Part II: *Thermodynamic performance simulation and design.* In: ASME Transactions, *Journal of Fluids Engineering* 119 (1997) 664.
4. Hanjalic, K., Stosic, N.: *Application of mathematical modeling of screw engines to the optimisation of lobe profiles.* In: Proc. VDI Tagung ''Schraubenmaschinen 94'' Dortmund VDI Berichte Nr. 1135, 1994.
5. Sauls, J.: *The influence of leakage on the performance of refrigerant screw compressors.* In: Proc. VDI Tagung ''Schraubenmaschinen 94'', Dortmund VDI Berichte 1135, 1994.
6. Stosic, N., Hanjalic, K.: *Development and optimization of screw machines with a simulation model.* Part I: *Profile generation*, In: ASME Transactions, Journal of Fluids Engineering **119** (1997) 659.
7. Stosic, N., I.K., Kovacevic, A.: *Optimization of screw compressor design.* In: XVI International Compressor Engineering Conference at Purdue, July, 2002.