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SIMULATION OF A WORKING CYCLE
OF MICRO RECIPROCATING COMPRESSORS

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ABSTRACT

Today, technology that permits devices and machines to be fabricated in micro sizes is readily available. Similar technology has benefited the development of micro-compressors. This paper describes a simulation approach of a complete working cycle of a micro-compressor taking into consideration of micro flow features. The treatment for the micro-compressor using the available findings in the literature related to MEMS together with an approach that has been developed will be proposed. The prediction on the P-V histories will be shown and discussed.

INTRODUCTION

Nanotechnology [1] has the potential of not only revolutionaries the whole manufacturing industry and materials processing, it has also changed the way we think, greatly, especially those related to engineering design. The miniaturising of energy systems, in particular, influences every aspect of engineering sciences to the extent that the existing theories and conventional fabrication techniques are greatly challenged. Today, the miniature devices or MEMS such as micro-engine, micro-motor, micro-turbo machinery and micro pump can be fabricated with relative ease. However, for air pumping applications, the development of high-pressure compressors has rarely been reported.

Steme E. et al [2] presented a piezoelectric micro-pump using diffuser nozzle element. Though the use of the diffuser valve instead of check valve simplifies the fabricating process of the micro-pump, at the same time, it penalizes the operating pressure range of the compressor. The use of the piezoelectric element as the "diaphragm" type compressing mechanism in this manner has also restricted the maximum pressure achievable. Fujiwira et al [3] developed a reciprocating air micro-compressor using a needle as the piston. Because of the use of a relatively large reciprocating motion generator, the combined compressor-prime mover, excludes the whole unit to be classified as a micro-compressor.

In a true sense of micro-compressor, the dimensions, in particular the characteristic dimensions such as the piston diameter should be within micro-scales. It is believed that the operation and the responses of such a small machine will be greatly different from the conventional ones. The applicability of conventional governing laws and theories in these micro-situations requires re-examination. Hitherto, all the simulation involving compressor at various levels of comprehensiveness such as the thermodynamics and the fluid dynamics description were normally carried out separately and the hypothesis of continuum mechanics was assumed. The latter is a reasonable assumption as the characteristic dimensions of these machines are relatively large as compared to the mean free path of the working medium. However, as the dimensions of the compressor reduce, rarefied and surface effects, viscosity and others are becoming more significant. When the dimensions of the compressor reached the micro-level, the mean free path is no longer negligible as compared to the characteristic dimensions of the flow geometry, hence descriptions by continuum mechanics failed. Under such situations, the flow is best described by kinetic theory of gasses and Navier-Stoke equation should be replaced by Boltzmann equation. Consequently, kinetic theory must combine with thermodynamics in order to give satisfied description of fluid behaviour, especially when the gas equation of state (Boyle's law or other equation of real gas) can't satisfy micro-scale behaviour of fluid.

Literature shows that the simulation of a whole working cycle for a micro-compressor taking into consideration of micro-features has not been reported. In fact, the true sense of micro-reciprocating compressors has not been developed. In this paper, an attempt has been made to introduce a new theoretical description of the working cycle of a micro-reciprocating compressor.

CONSIDERATIONS FOR MICRO-SIMULATION

Description form of a micro-compressor working cycle

Although both molecular dynamics (MD) and Boltzmann equation (BE) can be used to describe micro-scale systems, representation method of classical thermodynamics (property diagram) is more straightforward than statistical thermodynamics. From macroscopic viewpoint, the size of a reciprocating compressor is infinitesimal, but the space is very large when compared to the size of molecules of the working fluid i.e. one square micro volume contained several millions of molecules, hence representing a complete working cycle by macroscopic quantity has far-reaching significance.

The relationship between rarefaction and microflow

Rarefaction effects mean pressure drop, shear stress, heat flux and the corresponding mass flow rate can no longer be predicted using the flow and heat transfer model based on continuum hypothesis [4]. From a conventional definition [5], rarefied gases mean very low-density gases or low-pressure gases.

In the field of microelectromechanical systems (MEMS), Kn (i.e. mean free path/ characteristics dimension) may be large, which represents the degree of rarefaction effect. However, it must be noted that rarefaction effect in micro-geometry does not necessarily warrant the application of the rarefied gas theory. In fact, to the contrary, the application of such theory is inappropriate. This is because the reason for high Kn in the micro-sized geometry is a result of a size reduction while molecular density and hence the gas density remains constant. Under such a situation, an application of rarefied gas theory may not be suitable.

Consider this example: A house is with twenty persons distributed evenly. To illustrate the reduction in size from macro to micros, take only one tenth (in volume) of the size of the house and it should include two persons in this small space. Notice that the density does not change, the number of molecules per unit volume also remains constant. At the initial instant, in a full-scaled house, a person will interact with nineteen other persons, later with only one! Obviously, the behaviour of the "person" for these two cases will be different.

From this example, the gas with rarefaction effect behaves as if a person is placed in a prison normally with a very limited space. Under such a situation, the gas with rarefaction effects (NOT rarefied gas) and other effects such as compressibility, viscosity etc. should be re-examined because of variation of physical environment (size, boundary condition) and interaction between molecules. Hence, the rarefaction effect is obvious in micro-geometries, the gas within micro-scale compressor is not a rarefied gas if the conventional definition of rarefied gas is acknowledged. However, if Kn is the only determining factor, then the gas within the micro-scale compressor could easily be taken as a rarefied gas.

The gas in the micro-domain creates non-continuum phenomenon

In the continuum model, the gas is approximated as a continuous substance, with only the averaged effects of all the molecules in a finite region of the gas being considered. When rarefaction effects increase and characteristic size reduces, the interaction (though much less) between molecules becomes dominant. This dominating molecular motion results in a significant deviation of gas characteristics from the continuum description and that the continuum model fails. This deviation from the continuum behaviour is caused by two main reasons: First, the intermolecular interaction is greatly reduced because the total number of molecules is much less than that in macro-devices. Secondly, from the point of view of the derivation process of continuum kinetic equation, the micro-unit volume used by the computational

process of gas dynamics equation is so small that every micro-unit volume includes only a limited number of molecules, which is unsuited for continuum description. In other words, the molecular chaos restriction breaks down in the micro-computational volume, which is the prerequisite condition for the requirement of accurate computation of the macroscopic quantities (such as temperature and pressure) using the microscopic information [6].

The relationship between continuity and equilibrium

Continuity indicates the mathematical description form of flows, while equilibrium represents the state of the fluid. From the continuum viewpoint, the velocity distribution function of fluids is everywhere at the local equilibrium. If the fluid is not a continuous medium, the instant local equilibrium fails, the kinetic equation will describe this evolution physical process from non-equilibrium to equilibrium (local). Therefore, although continuity is closely related to equilibrium, the two have different significance [7].

The characteristic time and length scale difference between micro and macro domains

Mean free path is the average distance traveled (at constant velocity) by molecules between collisions. The mean free path time is the average time lapsed between two consecutive collisions of a given particle. The length of the mean free time and path determines the transition to local equilibrium. The evolution process in micro-domain is described by kinetic theory. The characteristic relaxation scales in the kinetic theory are the free path time and free path length.

One shall distinguish between the relaxation time of kinetic stage which leads to local equilibrium and the relaxation time governed by the gas dynamics process. In kinetic stage, the characteristic time is expressed in terms of internal parameters of the system, whereas in gas dynamic process the relaxation time depends on the external scale, for instance the dimensions of the system [8]. Although gas dynamic description corresponds to local thermodynamic equilibrium, the characteristic length and time scale between kinetic theory and gas dynamics is greatly different, hence different iteration time step in computation should be used when considering macro and micro problems. This will be discussed in the following sections.

The state settling time from non-equilibrium to equilibrium is longer in microscale than that in macroscale

When dealing with a non-continuum flow situation, the system settling time from a non-equilibrium state to reach an equilibrium state becomes an important parameter because the system takes more molecular collisions to reach the equilibrium as compared to continuum systems.

The total number of molecules within a micro-channel is significantly reduced as compared to the macro-ones implying that the collisions between molecules are less and less frequent than before. There is a need for time of evolution towards a most equilibrium state according to Second Law of Thermodynamics, hence the flow approaches the local equilibrium state in a relatively longer time as compared to those in low Kn. The equilibrium state here refers to the most randomized/chaotic state of gas molecules.

The relationship between the iteration time step and the settling time

The collision time is the time comparative to mean free path time; the iteration time step is the time interval used for computing the settling of the process. The settling time is the time for the micro-system to reorganize itself from one non-equilibrium state to an equilibrium state (local), which is the parameter that the iteration time step depends upon.

In the computation for a micro-compressor cycle, if every process within a small iteration time step is assumed as an evolution process from non-equilibrium to equilibrium, then the whole micro-compressor cycle can be simulated by replacing the complete continuous cycle with many discrete micro-processes. Therefore, the relationship $\Delta T_{iteration\ step} \geq \Delta T_{settling\ time}$ should be satisfied in order to guarantee the accuracy of the computation because the

process within the minimum time interval that the evolution equation can describe is $\Delta T_{settling\ time}$ at a given condition. If the settling time is known, then the iteration time step can be decided accordingly.

Feasibility of combining micro and macro-scale simulation approaches

In general, thermodynamics [18] can be divided into the probabilistic and the deterministic. The statistical thermodynamics belong to probabilistic, which links microscopic with macroscopic phenomenon, while deterministic thermodynamic does not consider the molecular structure of medium. The latter uses the macroscopic quantities to describe the state of the system [16]. BE and MD resemblance the statistical thermodynamics, which could bridge between microscopic and macroscopic phenomenon. BE as a tool for describing the micro-domain phenomenon pertaining to gas flow plays an important role in the simulation of micro-compressors. MD is the technique used in the present study involving the solution of the equation of motion or system of molecules that interact with each other through intermolecular potential. The MD method is not based on kinetic theory, but attempting to model such processes in molecular media as free motion and interaction of molecules, which is very useful for investigating flow from the microscopic viewpoint.

In the field of MEMS, the methodology of statistical thermodynamics and classical thermodynamics may be linked together because the micro regime is the transitional regime from macro-scale to molecular level.

PROPOSED MODELLING APPROACHES

The regime of micro reciprocating compressor

The working medium always exists as a gas phase in the compressor, whose degree of rarefaction is indicated by Kn. As an example to gauge the range of Kn, take the diameter of the cylinder of a micro-compressor as D while mean free path, L is 5×10^{-8} m (for air at the standard atmospheric condition P=1atm, T=298K). If D is between 0.1µ m and 10µm, Kn, which is L/D, will be between 0.005 and 0.5. Often, the Kn regime is ranged as follow [10]:

$$10^{-3} \leq Kn \leq 10^{-1} \quad \text{slip boundary condition}$$

$$10^{-1} \leq Kn \leq 10 \quad \text{transition regime}$$

Hence Kn of air in the micro-compressor is between 0.005 and 0.5, and it lies within the slip boundary condition and the transition regime. For other conditions and working medium of refrigerant, similar estimations can be made.

Current Simulation Method for Micro-Scale Devices

Generally, when the quantum effect is not appreciable, the mathematical modeling of working fluid in micro-devices can be described by three methods. These are Molecular Dynamics (MD), Boltzmann Equation (BE), direct simulation of Monte Carlo (DSMC). BE method belongs to statistical mechanics or kinetic theory, MD represents the molecular characteristics by classical mechanics law, while DSMC based on BE or MD, often used to compute fluid flow and heat transfer of rarefied gas. Each of the methods has its own merits and shortcoming.

MD method [11,12] requires a large amount of computational time, thus it may not be practically feasible for gas flows in MEMS. And, also that the molecular interaction is very important in this method but the molecular interaction are infrequent when Kn number is large. In the transition regimes, the kinetic theory of rarefied gas is more suitable, and BE can be solved if the nonlinear collision integral is simplified. DSMC is related to real physical time and is a statistical computational approach used to solve rarefied gas problems, and it is valid for all ranges of Kn [7].

Three Proposed Simulation methods

I. State Equation method

This method attempts to build a new equation of state (EOS) for micro-systems. Previous work based on First Law of Thermodynamics depends on equation of state to link pressure, temperature, thermodynamic property, and other state variables. For micro systems, a new EOS should be introduced using a new formulation suitable for micro-domains.

Π Kinetic Theory

From BE, the gas dynamics equation and equation of state (such as Boyle's law) can be derived, and the First Law of thermodynamics can be used in the micro-unit volume during the process of derivation. Hence, it is possible to combine the kinetic theory and the First Law of Thermodynamics to simulate the working cycle in micro-compressors.

1. Solve the Boltzmann equation directly

The whole cycle will be divided into many time intervals (iteration step for the complete working cycle), within which the evolution process is described by Boltzmann equation. The evolution process is simulated at every time interval (as if previous Navier-Stokes equation in dynamics simulation), by changing initial condition, boundary condition and Kn or other parameter. The boundary condition can be specified by flow rate of the working fluid and the temperature of the cylinder wall.

2. Expansion methods (combing the kinetic theory with the First Law of Thermodynamics)

In this approach, the kinetic theory can be used to describe the fluid flow in the micro-compressor, which obeys the First Law of Thermodynamics. The approach [13] here is to replace every terms in the First Law with functions describing the velocity distribution of the molecules to simulate the whole working process.

In this approach, the macroscopic quantity and gas property (pressure, work, temperature, internal energy, heat transfer) will be represented by velocity distribution functions.

Ш. Combination of DSMC and First Law of Thermodynamics

This method uses similar principle as that in method Π, the difference is that Boltzmann equation is substituted by DSMC.

Table 1 Differences between macro and micro compressor simulation method

Different section of simulation	Macro-compressor	Micro-compressor(MEMS)
Thermodynamic process	Classical thermodynamics	Combination of kinetic theory Related to statistical thermodynamics
Valve dynamics	Macro-valve	Micro-valve
Motion equation for the volume variation	Determined by conventional drive method	Micro-actuator
Heat transfer	General empirical correlations	Micro heat transfer consideration
Mass flow	Quasi-adiabatic flow through an orifice	A micro-orifice flow process

The method utilizing the Boltzmann equation (pertaining to method Π)

Since Kn in the micro-compressor indicates that the flow will be within the slip-boundary and the transition regime, therefore MD simulation and gas dynamics are not suitable, as mentioned before. Under such a situation, Boltzmann

equation or other kinetic evolution equation such as Liouville equation in the regime of slip boundary and transition would be more suitable. Boltzamnn equation describes a set of identical physical particles modeled as point masses and is in the intermediate position between the continuum theory of fluid dynamics and the discrete modeling of numerous numbers of particles by means of classical dynamics.

This section introduces the simulation process using Boltzmann equation and its solving method.

1. The mathematical model of working fluid

A general form of Boltzmann equation [14-19] with external force is

$$\frac{\partial f}{\partial t} + \xi \frac{\partial f}{\partial \vec{x}} + \frac{X}{m} \frac{\partial f}{\partial \xi} = I(f,f) \tag{1}$$

where

$X = (X_x, X_y, X_z)$ the external force which acts on a molecule with a mass

$f(t, x, \xi)$ the distribution function

$\vec{x} = (x, y, z)$ position vector

$\xi = (\xi_x, \xi_y, \xi_z)$ the velocity vector

$I(f, f)$ the collision integral operator, which account for the dissipation due to redistribution of particle's velocities because of interaction (collision) between two particles.

2. Boundary conditions and initial value

The initial condition has the form $f(0, \vec{x}, \xi) = f_{initial}(x, \xi)$, where $f_{initial}(\vec{x}, \xi)$ is function for $x \in V$ (physical space), restriction on the term of $f_{initial}(\vec{x}, \xi)$ should be determined by the appropriate existence theorems of the problem under consideration.

A solution to the Boltzmann equation is sought in the infinite domain of the velocity space and in the domain (finite or infinite) V of physical space bounded by a surface. The boundary can be divided into two parts, correspondingly respective to the boundary of the external flow and the surface of a body.

In the typical boundary conditions for a part of the Boltzmann equation (e.g. for a free boundary surface), if boundary condition function describes the undisturbed outer flow, the equilibrium distribution function for velocity ξ of equilibrium directed into the domain *V* is expressed as Maxwell distribution or others.

3. Selection of computation method for solving Boltzmann equation

At present, there are many methods of mathematical approaches to solving Boltzmann equation, which are often divided into analytical and numerical ones. Discussion about these methods is beyond the scope of this paper. However, it should be mentioned that the approximation of the distribution function and collision integral is the fundamental train of thought by whatever methods, because this function is the basis for computing macroscopic quantity or the quantity able to describe microscopic domain, transport coefficient, and other fluid property parameters.

4. The initial condition and boundary condition for a reciprocating micro-compressor

For the suction and discharge processes, the physical boundaries and outer flow boundary condition are coexist, while other processes only involve physical boundaries for describing the boundary conditions. The first initial condition may be assumed at a given equilibrium state, the initial condition of other iteration step is subsequently obtained from the results of the previous time step, as in the normal time marching problems, while the form of collision integral must be taken into account carefully.

5. The process of computation

In the First Law of Thermodynamics for closed systems, Q=W+ΔU , heat transfer and internal energy terms depend on the temperature of the working fluids, and work done is related to pressure of fluids and the displacement of the piston. Thus, the solution of pressure, P and temperature, T is the key to solving the problem for conventional simulation. In the micro systems, the condition is different, the macroscopic behavior cannot be described easily by the conventional quantity, instead, the distribution function will replace those quantities as a medium, and hence the iteration process will also be different.

As mentioned above, the method Π is categorized into two methods. One method is obtaining the value of the state variable such as P and T by computing the velocity distribution function through a direct simulation of Boltzmann Equation at every time interval. Because Kn determines the degree of rarefaction and validity of the continuum of the model, Kn changes with time and influences heat transfer and work. In order to solve this problem, as Kn, volumetric quantity (work) and boundary condition vary, the coefficient and boundary condition of Boltzmann equation will be decided at every iteration time step, the initial condition of subsequent time step is obtained from the equilibrium solution of the last time step.

In the situation that the First Law of Thermodynamics is employed together with the kinetic theory to simulate the working cycle of the micro-compressor, three fundamental considerations must be examined. First, what are the time dependent parameters? Secondly, what are the iteration procedures to be used and how to represent every term in the First Law properly? Thirdly, how to decide the initial and boundary conditions at every iteration time step? Alternatively, every term of the First Law of thermodynamics could be expressed in terms of approximation function of the velocity distribution. In this way, the velocity field is first computed, the value of pressure and temperature can then be calculated.

Physical explanation of the working cycle

In a compression cycle of a micro-compressor, it includes four processes: suction, compression, discharge and expansion. During these processes, the rarefied gas effect is significant. In the suction and discharge processes, the mass transfer rate is not zero, the flow situation may be modelled as flow through microchannel. However, for the compression and expansion processes since they involve no mass transfer (consider perfectly sealed systems), the compressibility, viscosity and other unconventional micro flow effects must be considered.

As the rarefaction effect increases, the interaction between molecules decreases, the gas can thus be compressed easily using less work. If less work is done, the heat transfer quantity will be reduced and less entropy will be generated. Thus, the gradient of the expansion curve is thus steeper for micro-compressor than that for the macro one. Inversely, the gradient of the compression curve is lower, see figure 1. Figure 1 is the predicted form of the PV histories for the micro and macro compressors.
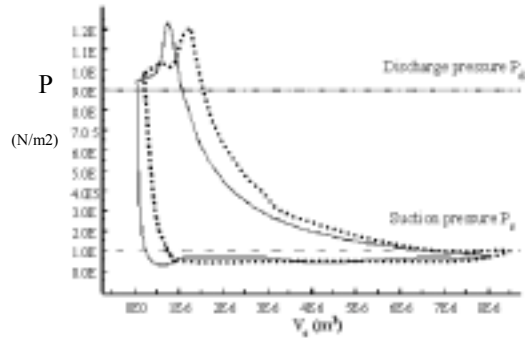
Figure 1 Comparison between PV histories of macro and micro compression cycles

In the diagram, the dot line represents P-V curve of macro compressor whereas the continuous line represents predicted curve of the micro compressor. In this figure, the PV diagram for the microcompressor is enlarged to fit the scale for the purpose of comparison. The qualitative variation of the parameters pertaining to four processes is shown in table 2.

Table 2 Variation of parameters during a compression cycle.

	Temperature	Molecular free path, Kn	Pressure	Volume
Expansion	↓	↑	↓	↑
Suction	↓	↓	Small variation	↑
Compression	↑	↓	↑	↓
Discharge	↓	Small variation	Small variation	↓

The properties of working fluid such as temperature and pressure are the average values within the whole cylinder, and simulation of valve dynamics, heat transfer, mass flow [10,20] etc. is not presented and will be the subject for future publication.

CONCLUSION

This paper presents feasibility of simulating a complete working cycle for a micro reciprocating compressor. Several possible methodologies are suggested and discussed. The method related to Boltzmann equation is focused upon, and the computation process is illustrated.

Following the arguments and elaboration presented, the predicted complete working cycle for the micro-compressor is shown together with that of the macro one on a PV history. The method presented in simulating the micro-reciprocating compressor is in fact applicable to simulating other fluidics involved in working cycle of fluid flow.

REFERENCES

1. Richard Feynman, Infinitesimal Machinery, Journal of Microelectromechanical Systems, Vol 2, No. 1, March 1993, pp 4-14.
2. Steme E. and Stemme, G., A Novel Piezoelectric Valveless Fluid Pump, Technical Digest of Transducers, pp 110-113,1993.
3. Mitsuru Fujiwara, Toshiharu Kazama, Yasahro Gunji, Reciprocating Air Microcompressor, Proceedings of International Compressor Engineering Conference at Purdue, Vol 1, pp 43-48, 1996.
4. Ali Beskok, George Eim Karniadakis, William Trimmer, Rarefaction and compressibility effects in gas microflows, September 1996, Transactions of the ASME, Journal of Fluids Engineering, Vol 118, pp 448-456.
5. James E. A. John, Gas Dynamics, Second Edition, 1984, Prentice-Hall Inc.
6. A. K. Bird, Molecular Gas Dynamics and Direct Simulation of Gas Flows, Clarendon Press, Oxford, 1994.
7. Mohamed Gad-el-Hak, The Fluid Mechanics of Microdevice –The Freeman Scholar Lecture, ASME Journal of Fluid Engineering, Vol 121, March 1999, pp 5-33.
8. Katja Lindenberg, Bruce J. West, The Nonequilibrium Statistical Mechanics of Open and Closed Systems.
9. W. Mus Chik, Nonequilibriun Thermodynamics With Applications Solids, Springer-Verlag, 1984.
10. Ali Beskok, A Model for Flows in Channels, Pipes, and Ducts at Micro and Nano Scales, Microscale Thermophysical Engineering, 1999, pp 43-77.
11. M. P. Allen, D.J. Tildesley, Computer Simulation of Liquids, Clarendon Press, Oxford Science Publications, Springer-Verlag.
12. Oblika C. Nwobi, Lylo N. Long, Michael Micci, Molecular Dynamics Study of Properties of Supercritical Fluids, Journal of Thermophysics and Heat Transfer, Vol 112, 1998 No. 3, pp 322-327.
13. M. Hatakeyama, S. Sugano, A. Takaada, Application of Function Approximation Methods to Computational Schemes for Discrete Boltzmann Equation, John Harvey and Gordon Lord, Rarefied Gas Dynamics : Proceedings of the 19th International Symposium held at the University of Oxford, 25-29 July 1994, Oxford ; New York : Oxford University Press , 1995.
14. Cercignani, The Boltzamann Equation and Its Application, 1988, Springer-Verlag.
15. Carlo Cercignani, Mathematical Methods in Kinetic Theory, Plenum Press, Second Edition, 1990.
16. P. P. J. M. Schram, Kinetic Theory of Gas and Plasmas, Kluwer Academic Publishers, 1991.
17. V. V Aristov, Direct Methods for Solving the Boltzmann Equation and Study of Non-Equilibrium Flows, KLUWRE Academic Publishers, 2001.
18. W. Fiszdon, Rarefied Gas Flows and Experiments, Springer-Verlag, 1981.
19. Yu. L. K. Limon Tovich, Statistical Theory of Open System, Kluwer Academic Publishers, 1995.
20. Bjοrn Palm, Heat Transfer in Microchannels, Microscale Thermophysical Engineering, No. 5, 2001, pp 155-175.