Jestr

Journal of Engineering Science and Technology Review 13 (6) (2020) 159 - 165

Research Article

JOURNAL OF
Engineering Science and Technology Review

www.jestr.org

Comparison Between Dynamic Discrete Element Method and Static Discrete Element Method to Determine Neck Size Between Powders During Sintering Process

Anas Obeed Balod[1], Ziad Shakeeb Al Sarraf[1,*] and Ekhlas Ahmed Basheer[2]

[1]*Department of Mechanical Engineering, University of Mosul, Mosul, IRAQ*
[2]*Department of Electronics Engineering, Ninevah University, Mosul, IRAQ*

Received 5 November 2019; Accepted 10 November 2020

Abstract

Sintering plays a significant role on powder technology which produces a new solid product from powders using thermal energy. There are many parameters effect on sintering process such as: Temperature, time, size of particles, geometrical structure of the powders, composition of the powder, density of the powders. Discrete element method is the best method to simulate the behaviour of powders during sintering process. There are two styles of discrete element method used in this report such as dynamic method and Qusi-static method. In this research will be compared of two types for DEM to simulate sintering process between two powders. In this paper, the sintering process between copper powders was simulated using discrete element method. The contact and shrinkage ratios were used to show the behaviour of copper powders during sintering process, and it was made a comparison between two styles of discrete element method. Some parameters used in the simulation to know the impact of these parameters on sintering process.

Keywords: Discrete element method, sintering process, grain boundary and surface diffusion.

1. Introduction

Sintering is an important stage in powder technology operation and we need to understand the whole process of sintering in order to overcome many errors in experimental sintering process especially the diffusions between powders [1]. There are different types of numerical solution but discrete element method (DEM) is useful method which has been used in this study. In addition, there are two styles of discrete element method such as dynamics method used Newton's second law of rigid body and another Qusi-static method without used dynamics model. In this study had used two styles of DEM to represent the mechanism of sintering between two particles.

Bouvard and McMeeking (1996)[2] used finite difference method to simulate the sintering process between powders theoretically using two types of diffusions such as grain boundary and surface diffusion and comparing with analytical formula. They noted that the numerical results of neck size ratio and shrinkage ratio between powders have good agreement with analytical formula. Parhami F., R.M. McMeeking R.M.(1999)[3] simulated a model of the densification between spherical powders during early stage of sintering process via discrete element method using surface and grain boundary diffusion to show the behaviour between powders. Also they studied the effect of powder size, applied force, and dihedral angle. They displayed that the results has a good agreement with Coble's analytical [4]. Moreover, the neck size ratio increased with increasing dihedral angle.

Martin C.L. et al (2003)[5] simulated sintering process numerically using discrete element method to determine the behaviour of powders during process, and also they studied the rearrangement of powders. They compared with experimental results and concluded that the rearrangement of powders effected on contact between powders. Peng Chen et al(2008) [6] model the sintering process between powders using discrete element method, also they studied the effect of force and temperature of powders during sintering process. They concluded that the numerical results had good agreement with Exner (1979) [7] experimental results. Nosewicz S. et al (2013) [8] simulated the solid state sintering process for viscoelasticity model using discrete element method for different types of material. They discovered that the numerical results via viscoelasticity model matched with experimental results.

Yan.Z et al (2014) [9] simulated the multilayer of composite during co-sintering process using discrete element method to investigate the influence of heat rate, rearrangement, density and thickness. They concluded that the electrode discontinuity decreases with increasing heat rate, and the connectivity of the electrode enhanced via rearrangement of powders. Martin et al (2015) [10] simulated the bimodal powders using a discrete element method, and also they studied the effect of the contact type of powders. They concluded that the contact ratio depending on contact types and size.

The mechanism of sintering process between powders depends on the types of diffusions which controls atomic transport between powders. The grain boundary and surface diffusion represents basic mechanism to control atomic transport between powders [1].

In this research, the simulation of sintering process between copper powders are determined using two styles of discrete element method, and comparing between two styles to show the best style of behavior of powders during sintering process. The numerical results for both DE methods were

*E-mail address: ziad_sarraf@yahoo.com
ISSN: 1791-2377
doi:10.25103/jestr.136.22

compared with experimental and analytical results to check the numerical solution matches to real results.

2. Analytical formula for sintering process between powders

The first model of sintering between particles of grain boundary diffusion is proposed by Coble(1958)[4], after that, the model was corrected by Coblenz et al[11]. The equation (1) represents the correction model of grain boundary sintering.

$$\frac{a}{R} = \left(\frac{19 \cdot 2t}{\tau_g}\right)^{1/6} \tag{1}$$

and equation (2) represents τ_g

$$\tau_g = \frac{KTR^4}{\Omega \delta_g D_g \gamma_s} \tag{2}$$

3. Numerical models of sintering

There are different methods used to solve sintering between particles i.e. Finite element method, finite difference method, Monte Carlo method, Molecular dynamics method and discrete element method. The numerical solution of sintering is progressed with discrete element model which represents group of spherical particles contacting and affect one to another.

4. Discrete Element Method (DEM)

The Discrete Element Method (DEM) is a numerical technique used to calculate the forces, displacements and acceleration between particles in a shape containing a great number of particles such as powder. There are two styles of DEM to determine the sintering process between copper powders.

5. First Method: Dynamics method

Discrete Element Method (DEM) is any group of numerical techniques that used for calculating the motion of a big number of particles for different scale sizes. DEM is very nearly interconnected to molecular dynamics. Nowadays, DEM is reaching widely agreed as an active method to solve engineering problems in granular and discontinuous materials, especially in granular, powder, and rock mechanics. Although the method was initially used by scientist's researches in Mechanics of rock, but it has effectively been applied to model micro structural evolution. The movement of solid particles is defined by the Newton's second law of rigid body dynamics.

$$m_i A = F_i \tag{3}$$

where m_i is the mass of particle; F_i is the sum of all the forces, and F_i is represent two types of force which first external load F_{ex} and second contact force with neighbouring particles F_{ijc} [15].

$$F_i = F_{ex} + \sum_{j=1}^{n_i^c} F_{ijc} \tag{4}$$

The model represents bond between two particles during free sintering. The classical model was developed by [15, 16, 17] and was actually used in pervious applications of the discrete element method. The normal force (F_n) between two spherical particles for same radius (R) is given by the equation (5) which equal two forces such as viscous resistance force (F_v) and the sintering force (F_s).

$$F_n = F_V + F_s \tag{5}$$

The viscous resistance force (F_v) is given by equation (6), and the sintering force (F_s) is given by equation (7)

$$F_V = \frac{\pi a^4}{8 D_b} V_n \tag{6}$$

$$F_S = \pi \gamma_s [4R(1 - \cos\tfrac{\Psi}{2}) + \operatorname{asin}\tfrac{\Psi}{2}] \tag{7}$$

Fig. 1 shows the effective geometry parameters in two particles sintering model.

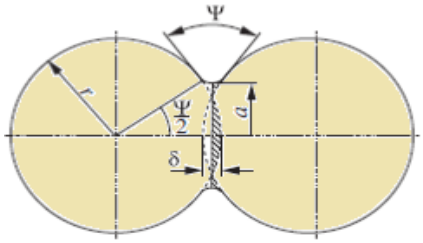

Fig. 1. geometry parameters of two particles sintering [8]

The effective grain boundary diffusion coefficient of vacancy movement between particles is given by equation (8)

$$D_b = \frac{\Omega}{kT} \delta_b D_{0b} \exp\left(-\frac{Q_b}{RT}\right) \tag{8}$$

The growth of neck radius of overlap between particles is controlled by coble's model using equation (9).

$$\dot{a} = -\frac{RV_n}{a} \tag{9}$$

The condition of complete sintering process between particles occurs when the neck radius (a) reaching maximum value (am) which gives by equation (10).

$$a_m = \frac{R}{2} \sin \Psi \tag{10}$$

It can be used for different sizes by changing particle radius (R) in all the equation with the effect particle radius (R_e) which is given by equation (11).

$$\mathrm{R_e} = \frac{2R_i R_j}{R_i + R_j} \tag{11}$$

The viscous sintering model can be represented by rheological outline shown in Fig. 2 [8].

6. Second method: Qusi-static model

The Qusi-static model focuses on bond between two neighboring particles during free sintering. This model was first used by Parhami F, R.M. McMeeking [14] to simulate the sintering between particles. In this model, the center of

particle is considered by a node, and any connection between two neighbouring particles by a discrete element method [14]. Fig. 3 shows the two dimensional of two powders connected together in a small position which known neck [13].

Bouvard and McMeeking (1996) proposed appropriate formula for the axial velocity of the particle centre [2].

$$V_n = \frac{8D_b}{a^2}[\sigma + \gamma_s K(r) - \frac{2\gamma s}{a}\sin\frac{\Psi}{2}] \quad (12)$$

where:

$$D_b = \frac{D_g \delta_g \Omega}{KT} \quad (13)$$

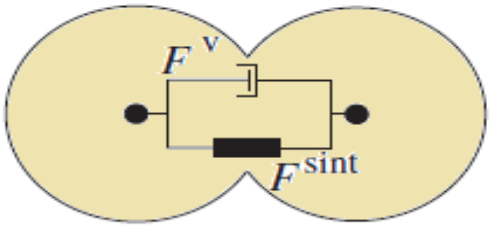

Fig. 2. rheological of viscous model [8]

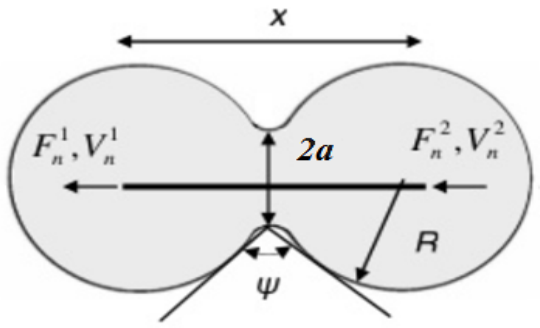

Fig. 3. Qusi-static model of two powders [13].

The summation of the curvatures is shown in equation (14)

$$K(\alpha) = -\frac{1}{S} + \frac{1}{a}\sin\frac{\Psi}{2} \quad (14)$$

Coble (1958)[4] has suggested that the model of the two spherical particles bonding by neck part with radius of free surface curvature S is constant.

$$\frac{1}{S} = [1 - \cos\frac{\Psi}{2}]\frac{4R}{\alpha^2} \quad (15)$$

Substitution of equations (15) and (14) into equation (12) gives equation (16).

$$V_n = \frac{8D_b}{a^2}\sigma - \frac{8D_b\gamma S}{a^4}[4R(1 - \cos\frac{\Psi}{2}) + \alpha\sin\frac{\Psi}{2}] \quad (16)$$

The rate of growth of neck radius is controlled by coble's model using equation (17).

$$\dot{a} = -\frac{RV_n}{a} \quad (17)$$

The normal applied stress on the inside particle grain boundary is given by equation (18).

$$\sigma = \frac{F_n}{\pi\alpha^2} \quad (18)$$

The equilibrium condition of complete sintering process between particles occurs when the neck radius (a) will reach maximum value (am) which gives by equation (19).

$$a_m = \frac{R\sin\Psi}{2} \quad (19)$$

7. Parameters input and computer code

Input parameters of copper powder

Copper and Alumina have been selected in this report. Table (1) shows the data of copper.

Table 1. Input parameters of copper used in numerical model [12, 18]

Parameter	Value	Parameter	Value
Specific surface energy γS	1.72 J/m^2	Initial particle radius R	22.5×10-6m
Specific grain-boundary energy γgb	1 J/m^2	Atomic volume **Ω**	1.18×10-29 m^3
Grain-boundary thickness pre-exponential grain-boundary diffusion coefficient δ**g**b D**g**bo	5.12 × 10-15m^3/s	Dihedral angle	146°
		Sintering temperature	1027°C
Gas constant Rr	8.3144621 J/(mol K)	Activation energy for grain boundary diffusion **Qg**b	1.05×105 J/mol
Boltzmann's constant k	1.3806503×10-23m^{2}kg/(s2K)		

Computer Programming

This study used Fortran program code to describe the two styles of the discrete element method (DEM) to solve sintering between particles in solid state. The flowchart of program of the dynamics style of DEM is shown in Fig. 4. Fig. 5 shows the flowchart of program of another style of DEM.

8. Results and discussions

The general condition of sintering simulation in this study is free sintering which means that the stress equal zero. Copper powders were used in numerical simulation, and parameters of these powders were used input in computer program. The viscous model has been used, and this model contains overlap between two sphere powders. Two styles of discrete element

method have been used in the numerical simulation such as dynamics and Qusi-static method. Neck size ratio plays an important role in sintering process because we can know sintering stages depends on this factor, and this factor equal the neck radius to powder radius. Fig. 6 shows the neck size ratio as a function of the sintering time for sintering between two copper powders, and this result has been achieved using the numerical model which represents qusi static method of discrete element method. The neck ratio significantly increases with increasing sintering time and reaches 0.4. After that, the curve slightly increases to the end of the curve. The figure also shows a very fast initial stage of sintering process comparing to the final stage.

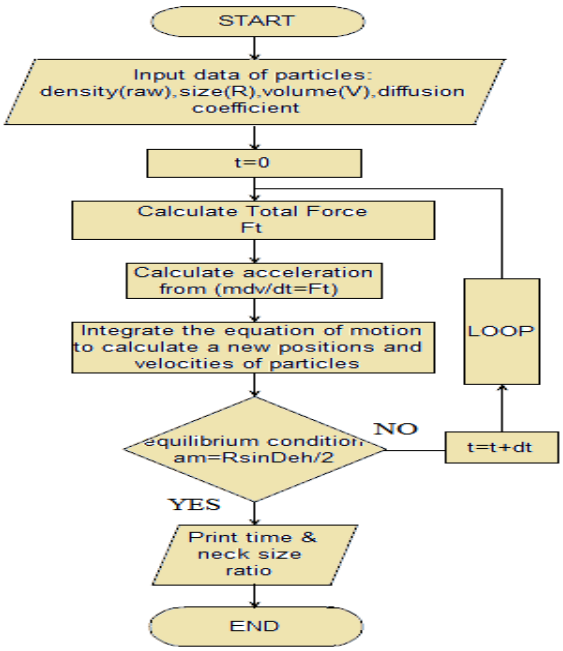

Fig. 4. flowchart of first style of DEM: Dynamics method

Shrinkage is define as the linear dimensional change ΔL/Lo which means that the change in the initial length to the final sintered length given as ΔL to original length Lo. Fig. 7 shows the shrinkage ratio as a function of the sintering time for sintering process between two copper powders, and this result was reached from numerical model which represented by Qusi-static method of discrete element method. Over all, the shrinkage ratio increases with increasing sintering time, and it can be seen that the maximum shrinkage ratio is 0.425 with sintering time 430 hr.

The surface area reduction, is define as the reduction in surface area ΔS/So which means that the change in the initial surface area to the final sintered surface area given as ΔS to original surface area So. Fig. 8 shows the surface area reduction with time curve of sintering between two copper particles, and this result was reached from numerical model which represented by qusi-static method of discrete element method.

Equation (20) was used in numerical model program to determine the surface area reduction, and the Particle coordination number NC is equal 2 which used as an input in the computer program. It can be seen that the surface area reduction increases with increased the neck size ratio. Moreover, the surface area reduction slightly increase in the initial sintering stage while sharply increase in the final sintering stage.

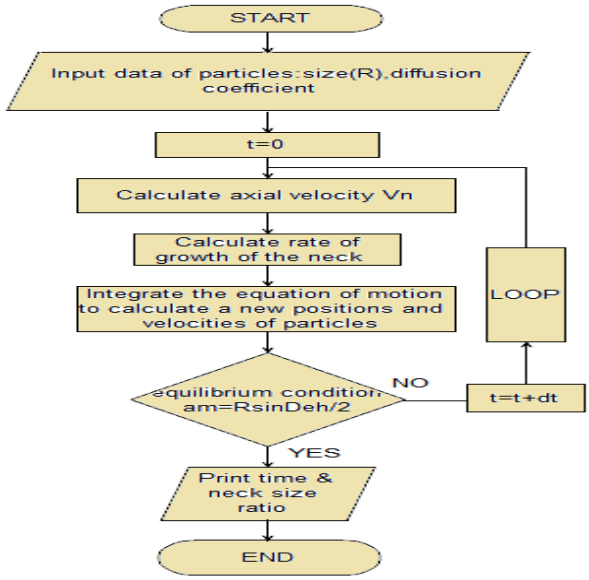

Fig. 5. flowchart of second style of DEM: Qusi-static method

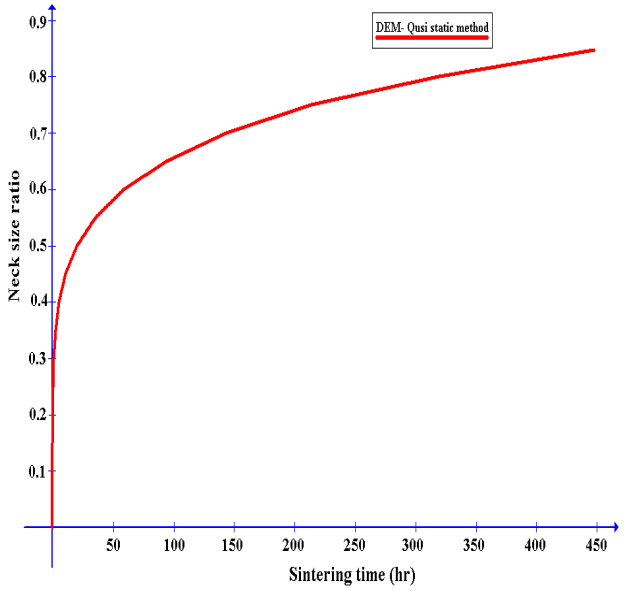

Fig. 6. neck ratio and time of copper for DEM Qusi static method

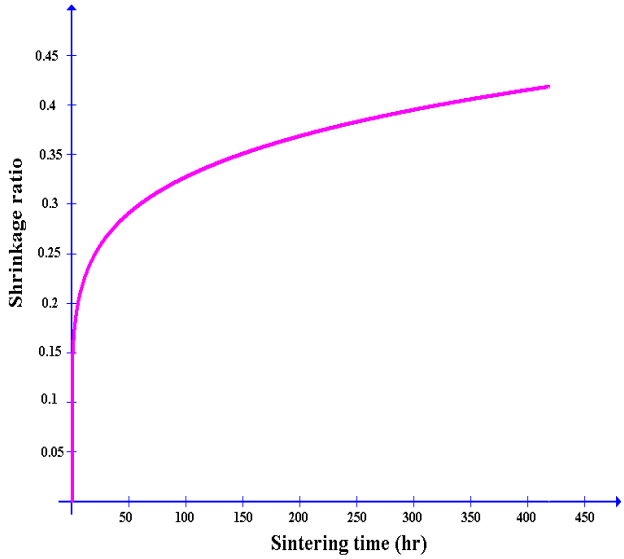

Fig. 7. the shrinkage ratio and time of copper particles for DEM- Qusi-static method

$$\frac{\Delta S}{S_O} = \frac{N_C}{4}\left(\frac{a}{R}\right)^2 \quad (20)$$

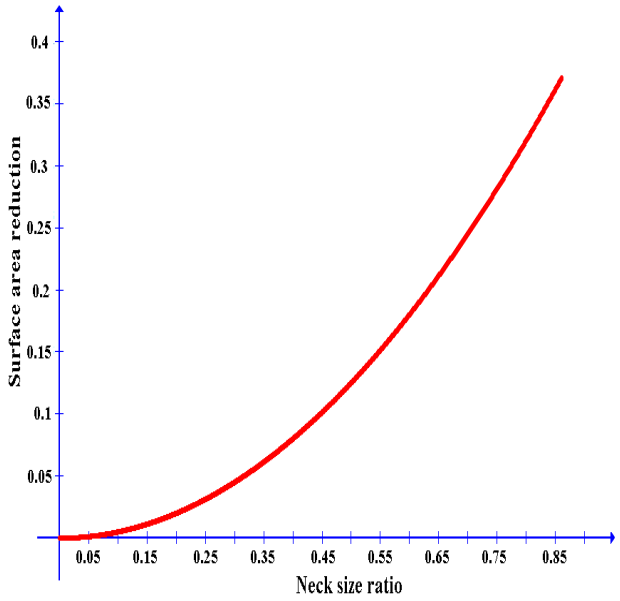

Fig. 8. the surface area reduction for copper powders

9. Effective parameter of sintering

Three general parameters have been used in numerical simulation to show the effect of each parameter on sintering process. The first parameter is dihedral angle which defines as an angle of contacting between two powders (see figure 9). Figure (10) shows comparison between three curves of different dihedral angles, and the vertical axis represents the neck size ratio and horizontal axis represents sintering time, this study used three different dihedral angles i.e. 130̊, 146̊ and 160̊. As can be seen, the impact of the dihedral angle is small effective on sintering process, when the dihedral angle is changed.

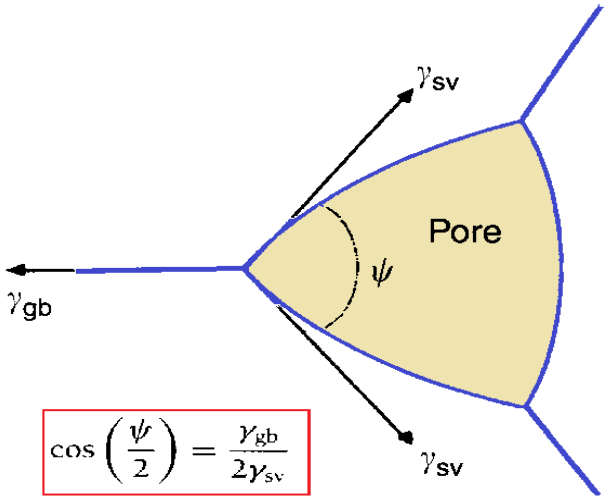

Fig. 9. Dihedral angle and balance energy

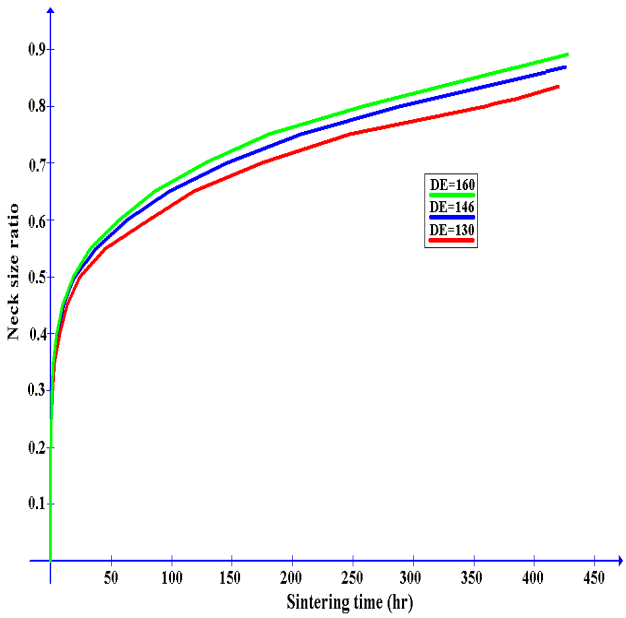

Fig. 10. comparison between three curves represents three different dihedral angles

Another important parameter is the size of the powder which uses in numerical program. Fig. 11 shows comparison between four curves of different particle sizes of copper particles, the vertical axis represents the neck size ratio and the horizontal axis represents sintering time. Four different particle sizes i.e. 9, 12, 18 and 22.5µm were used in this research to study the effect of particle size in sintering process. The sintering time increases with increased particles size but the sintering process is very fast when particle size is smaller

.

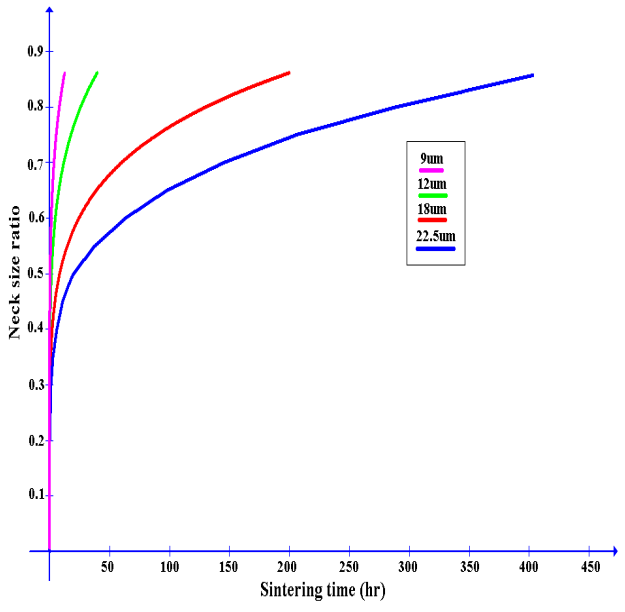

Fig. 11. comparison between four curves represents four different particle sizes

Sintering temperature is a significant parameter in sintering process. Fig. 12 illustrates comparison between three curves of different sintering temperatures of two copper particles. Three different sintering temperatures: 1100, 1200

and 1300℃ were used in this study to investigate about the effect of sintering temperature on sintering process. The sintering time increases with decreased sintering temperatures which mean that the sintering process is very fast by increasing the temperature.

10. Validation of Numerical Results

Coble (1958) [4] had constructed sintering model, and the model was corrected by Coblenz et al (1980) [11]. The final model became new formula in equation (3.7) which used in comparison with numerical simulation. Fig. 13 shows comparison between two different methods of discrete element model and analytical solution by Coble (1958) [4].

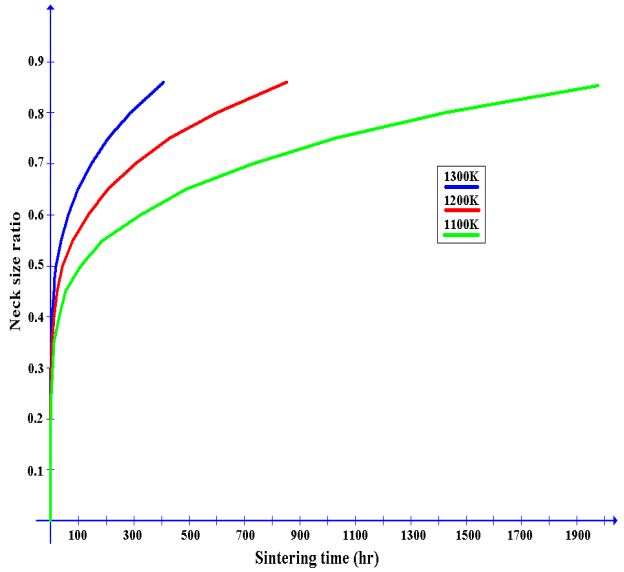

Fig. 12. comparison between three curves represents three different sintering temperatures

The analytical solution spends more time than numerical model but it close to the two curves; in addition, the curve of dynamics method is higher than two curves.

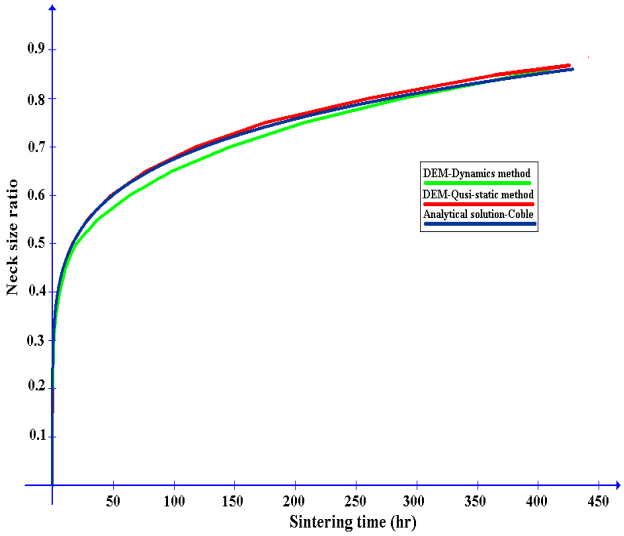

Fig. 13. comparison between two different methods of DEM and analytical solution by coble

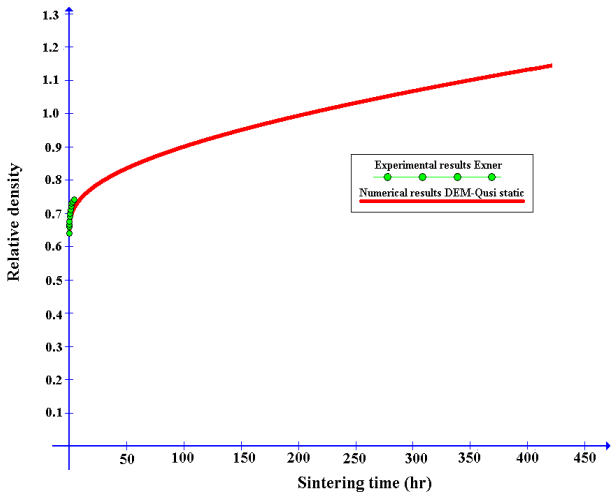

Fig. 14. comparison between numerical model and Exner's experimental

Exner (1979) [7] has used copper particles to make experimental sintering and to compute the relative density of particles. He analysed and drew the curve between relative density and time to show the behaviour of particles with time. Fig. 14 & Fig. 15 Shows a comparison between numerical model and experimental Exner's result of relative density with the time of sintering between two copper particles. Equations (21) & (22) were used in numerical model program to determine the relative density [8], and the initial relative density is equal 0.64 which used as an input in the computer code [12]. It can be seen from the two figures that the numerical model curve is close to the experimental Exner's curve.

$$\rho_r = \rho_0 \frac{1}{(1+e)^3} \tag{21}$$

$$e = \frac{\Delta L}{L_0} \tag{22}$$

Fig. 15 shows the comparison between numerical model and experimental Exner's result (1979). Exner's result is clear available for the early stage of sintering but the numerical results continue to the end of sintering process which is shown in Fig. 14, and the numerical results agree well with the experimental results.

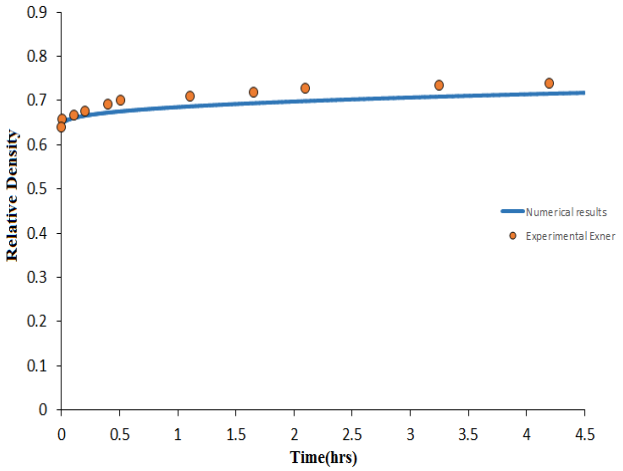

Fig. 15. comparison between numerical result of initial stage sintering and Exner's experimental [7]

11. Conclusions

This research focuses on simulation of sintering between two copper powders using two styles of discrete element method, such as, dynamics method and Qusi-static method. Firstly, the two styles of discrete element methods were compared using contact ratio to find the easier method of DEM. Secondly, Three parameters are used on simulation to study the effect of these parameters on sintering process between copper powders numerically.

My research clarified the following points:

1. In general, the contact ratio (neck radius to powder radius) increased with increasing sintering time.
2. The period of time for initial stage of sintering process is very fast comparing to the final and intermediate stages.
3. The Qusi-static method is easier than Dynamics method for applying of computer program.
4. The numerical results show the good agreement with analytical and experimental results.
5. The effect of the dihedral angle between powders is insignificant comparing with anther parameters.
6. The sintering time increases with increasing particle size whereas the sintering process becomes faster when particle size is smaller.
7. The sintering time increases with decreasing a sintering temperature which means that the sintering process is very fast by increasing the sintering temperature.

References

1. German RM. Sintering theory and practice. Sintering Theory and Practice, by Randall M German, pp 568 ISBN 0-471-05786-X Wiley-VCH, January 1996. 1996;1.
2. Bouvard D, McMeeking R. Deformation of Interparticle Necks by Diffusion-Controlled Creep. Journal of the American Ceramic Society. 1996;79:666-72.
3. Parhami F, McMeeking R, Cocks A, Suo Z. A model for the sintering and coarsening of rows of spherical particles. Mechanics of Materials. 1999;31:43-61.
4. Coble R. Initial sintering of alumina and hematite. Journal of the American Ceramic Society. 1958;41:55-62.
5. Martin C, Bouvard D, Shima S. Study of particle rearrangement during powder compaction by the discrete element method. Journal of the Mechanics and Physics of Solids. 2003; 51:667-93.
6. Chen P, Ni J. Discrete element modeling of micro-feature hot compaction process. Transactions of the North American Manufacturing Research Institution/SME.36.
7. Exner HE. Principles of single-phase sintering. Rev Powder Metall Phys Ceram 1,(1/4), 1979. 1979.
8. Nosewicz S, Rojek J, Pietrzak K, Chmielewski M. Viscoelastic discrete element model of powder sintering. Powder Technology. 2013; 246:157-68.
9. Yan Z, Martin CL, Guillon O, Bouvard D., Lee C.S., Microstructure evolution during the co-sintering of Ni/BaTiO3multilayerceramic capacitors modeled by discrete element simulations. Journal of the European Ceramic Society 34 (2014) 3167–3179
10. Martin S, Parekh R, Guessasma M, Léchelle J, Fortin J, Saleh K. Study of the sintering kinetics of bimodal powders. A parametric DEM study. Powder Technology. 2015;270:637-45.
11. Coblenz W, Dynys J, Cannon R, Coble R. Initial stage solid state sintering models. A critical analysis and assessment. Sintering Processes Materials Science Research. 1980;13:141-57.
12. Parhami F, McMeeking R. A network model for initial stage sintering. Mechanics of materials. 1998;27:111-24.
13. Chen P, Ni J. Discrete element modeling of micro-feature hot compaction process. Transactions of the North American Manufacturing Research Institution/SME.36.
14. Parhami F, McMeeking R, Cocks A, Suo Z. A model for the sintering and coarsening of rows of spherical particles. Mechanics of Materials. 1999;31:43-61.
15. Coble RL. Sintering crystalline solids. I. Intermediate and final state diffusion models. Journal of applied physics. 1961;32:787-92.
16. Johnson DL. New Method of Obtaining Volume, Grain-Boundary, and Surface Diffusion Coefficients from Sintering Data. Journal of Applied Physics. 1969;40:192-200.
17. De Jonghe LC, Rahaman MN. Sintering stress of homogeneous and heterogeneous powder compacts. Acta Metallurgica. 1988;36:223-9.
18. Martin C, Schneider L, Olmos L, Bouvard D. Discrete element modeling of metallic powder sintering. Scripta materialia. 2006;55:425-8.