Investigation on Parameter Identification and Coarse Graining Models using Discrete Element Capability in LS-DYNA

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1 Introduction

Processes such as transportation, flowing and processing of powder materials can be seen in the manufacturing process of various industrial products and are important processes for manufacturing high quality products. Discrete Element Method (DEM)[1] is widely used as a simulation method to handle powder materials, and excellent DEM function is also implemented in LS-DYNA. The DEM model can be used intuitively, and there is an advantage that stable computation can be performed. On the other hand, the DEM model is a hypothetical model based on the spring-mass model, and in order to reproduce the real phenomenon with high accuracy, it includes many numerical parameters that the user must decide beforehand. In this paper, the simulation of a compression experiment of polymer pellets were performed and the result of the parameter identification using optimization software LS-OPT is reported. In addition, when DEM is applied to fine powder material, the number of particles becomes enormous, and in many cases it cannot be processed in a common computational environment. In such a case, a coarse graining model is used to reduce the number of particles and computational load. Various ideas have been proposed for the method of coarse graining so far, and in this paper several coarse graining models were tested to compare powder behavior in drum mixing problem.

2 Parameter identification in simulation of polymer pellet compression

In a kneading process using a twin-screw extruder, solid polymer pellets are supplied, and the melted polymer is extruded. At the initial stage of this process, the solid polymer pellets are compressed. In order to study the possibility of modeling by DEM in this state, pellet compression experiments were carried out. As the result, pressure-volume relationship was obtained. Pellets with a diameter of 3.72 mm were filled in a cylindrical container having an inner diameter of 36 mm and a height of 64 mm, and the pellets were compressed from above by a piston. The material properties of the pellets are shown in Table 1. The spring stiffness of the DEM model K_{spring} can be determined using these properties and following definition;

$$K_{spring} = K_{bulk}*RADIUS*NORMK$$

where, K_{Bulk} is the bulk modulus which can be given by Young's modulus and Poisson's ratio and RADIUS is the particle radius. NORMK is the numerical parameter which should be determined to match with experimental results. DEM model in LS-DYNA has one more numerical parameter SHEARK which should also be determined. So, parameter identification was performed by curve fitting scheme based on Radial Basis Function (RBF) network using LS-OPT. The compression states of the simulation are shown in Fig.1. The results are shown in Table 1 and Fig.2. As shown in the figure, good agreement of the simulation result with the experiment could be obtained.

3 Comparison of coarse graining models

When very fine powder is modelled using DEM, coarse graining technique is necessary in most cases to reduce computational cost. There are several idea of the coarse graining models and the best of which is problem dependent. In this paper, referring to useful suggestion in [Karajan et al., 2014][3], the behaviour of powder using simple coarse graining model and coarse graining model considering volume fraction or porosity are compared in rotary drum simulation. In this paper, the simple coarse graining model and the coarse graining model with volume fraction are represented by the notation as "SCG" and "CVF" respectively. The definition of parameters shown in Table 2 are used in the simulation. An example of the rotary drum model is shown in Fig.3. The DEM particles are generated in a region enclosed by dummy shell elements using packed particle generation capability in LS-PREPOST. In this

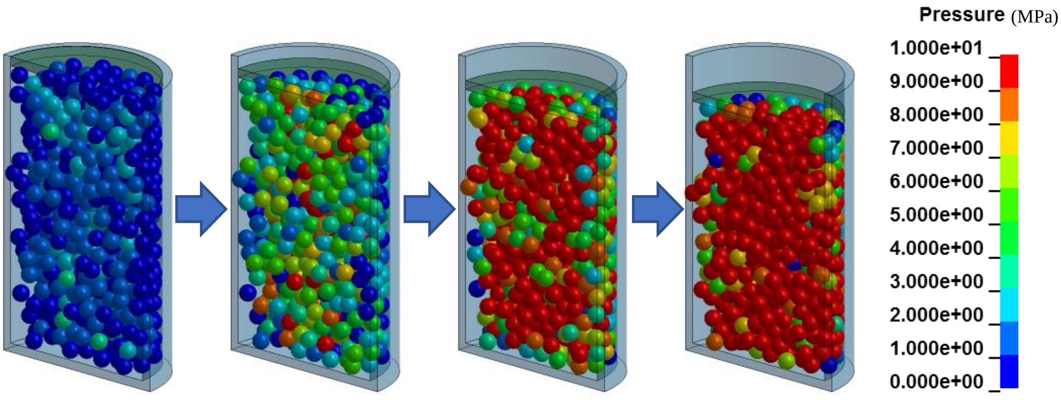

Fig.1: Simulation of polymer pellet compression (cross section view)

Parameter	Value
Young's modulus, E (MPa)	1,060
Poisson's ratio, ν	0.4
$K_{bulk}=\dfrac{E}{3(1-2\nu)}$ (MPa)	1,767
RADIUS (mm)	1.86
NORMK (default=0.01)	0.875046
SHEARK (default=2/7=0.2857)	0.299582

Table 1: Material properties of pellets and identified numerical parameters (NORMK and SHEARK)

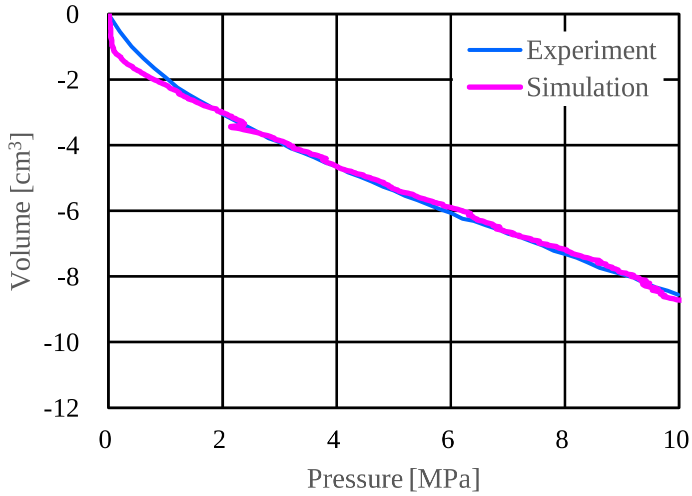

Fig.2: Pressure-volume relations for experiment and simulation

case, particles are not generated densely in the region. So the adjustment of the amount of the total mass (or the number) of particles to the desired value is required by extending the volume of the packed region. In addition, computation of densitification process of the particles are also necessary in early stage of the simulation. Many papers suggest that the typical volume fraction of randamly packed granular materials is between 0.6 and 0.7[4]. So the volume fraction $\phi = 0.64$ is adopted in this study.

The behaviours of particles which have the scale factor = 1 (original model), scale factor = 2 and scale factor = 4 in the rotary drum for both SCG model and CVF model are compared. The rotational speed of the drum is 60 RPM. The situations of the DEM particles in each case at the time of three seconds from the beginning are shown in Fig.4. Torque history curves of the drum are plotted in Fig.5 as the

	Simple coarse graining model	Coarse graining model with volume fraction
Radius of a particle	$r_{\mathrm{SCG}} = s r_0$	$r_{\mathrm{CVF}} = \phi^{-1/3} s r_0$
Volume of a particle	$v_{\mathrm{SCG}} = s^3 v_0$	$v_{\mathrm{CVF}} = \frac{1}{\phi} s^3 v_0$
Mass of a particle	$m_{\mathrm{SCG}} = s^3 m_0$	$m_{\mathrm{CVF}} = s^3 m_0$
True density of a particle	$\rho_{\mathrm{SCG}} = \rho_0$	$\rho_{\mathrm{CVF}} = \phi \rho_0$
Total mass of particles	$M_{\mathrm{SCG}} = M_0$	$M_{\mathrm{CVF}} = \phi M_0$

s ; scaling factor, ϕ ; volume fraction, r_0, m_0, r_0, M_0 ; radius, mass, density and total mass of original particle(s), respectively

Table 2: Definition of coarse graining models

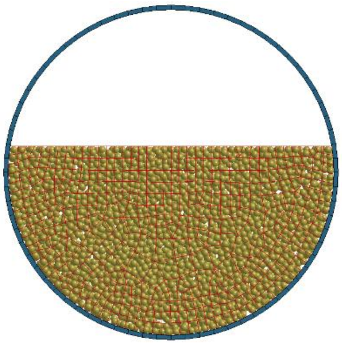

Fig.3: Example of generated DEM particles in the specified packed region

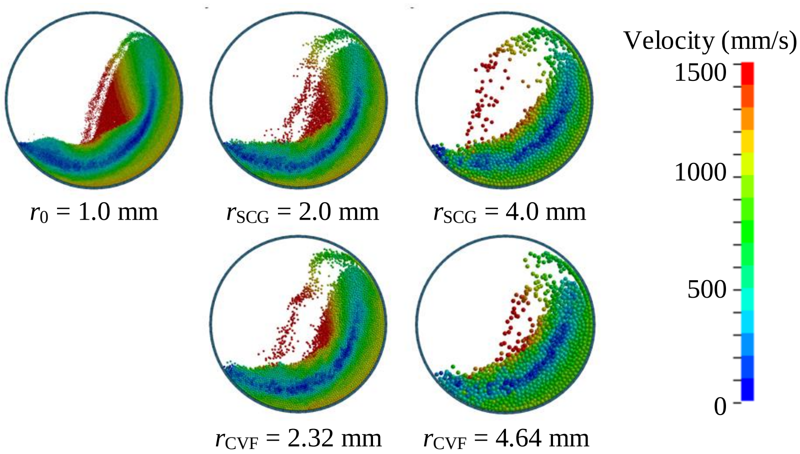

Fig.4: Comparison of shape of particles for the original, SCG and CVF model

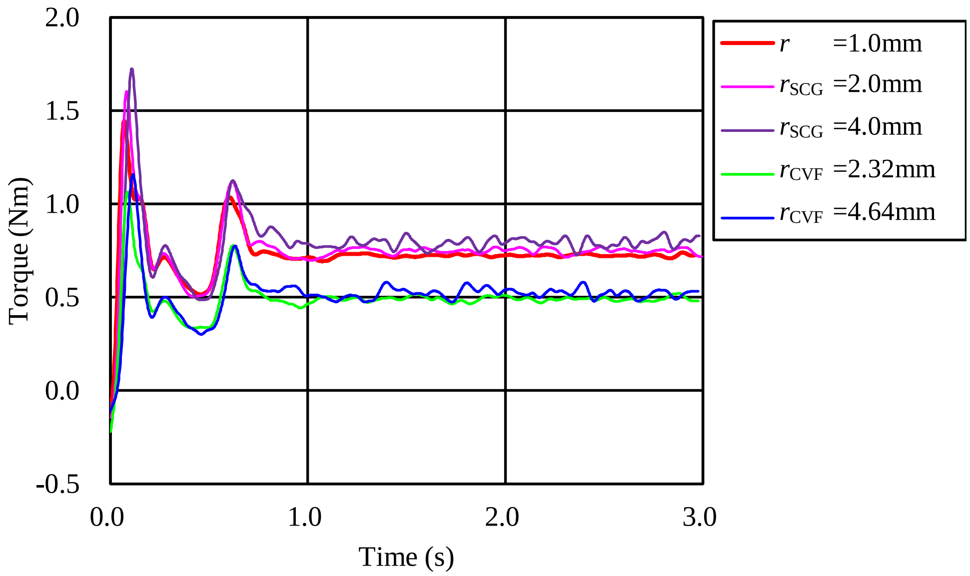

Fig.5: Torque (z-moment) of drum

torque of drum is also an important design factor for powder manufacturing. As seen in Fig.4, the behaviour of particles in the case of SCG model with radius = 4.0 mm is very different from the original one. Parameter identification for the coarse graining model is necessary to reproduce original powder behaviour in such case. So the parameter identification was performed using following procedure. The paper[3] suggests that identification of parameters, e.g., friction coefficients, should be performed by reference to repose angle shown in Fig.6. However, in many cases, repose angle cannot be seen clearly as shown in Fig.4. So, in this paper, curve fitting technique was used instead of repose angle to identify the parameters. First, surface curve of the powder in the original case was extracted manually from the deformed figure as shown in Fig.7. This surface curve is the target of the curve fitting. Second, multiple simulation of SCG model with r=4.0 mm was performed using LS-OPT. The surface curve of each simulation was extracted using simple program and compared with the target curve. Finally, optimal solution was obtained. The initial values and the optimal values of the parameters are listed on Table 3. Nine variables are selected for parameter identification and RBF network with space filling sampling method was adopted. 16 sampling points were used per iteration and 100 iterations (1600 computations) were executed. The optimal result of the parameter identification and fitted curve are shown in Fig.8. the minimum, the maximum and the average of CPU time per execution were 390 seconds, 4,688 seconds and 3,878 secons respectively. It is largely depends on the spring coefficient of DEM particle.

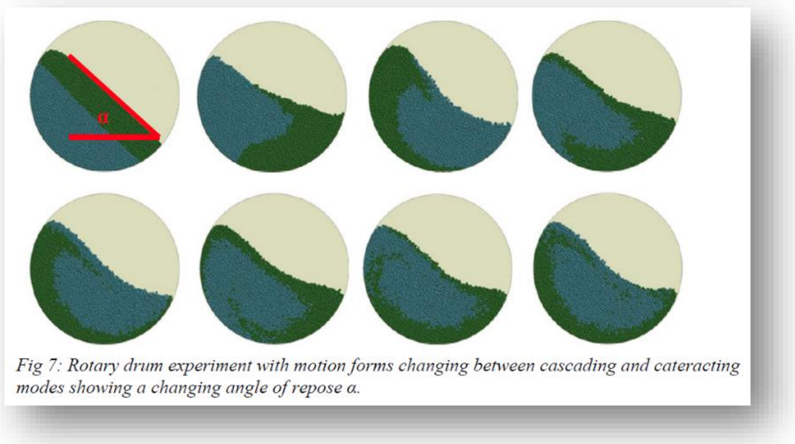

Fig.6: Repose angle which characterizes mixing behaviour of powder in rotary drum[3]

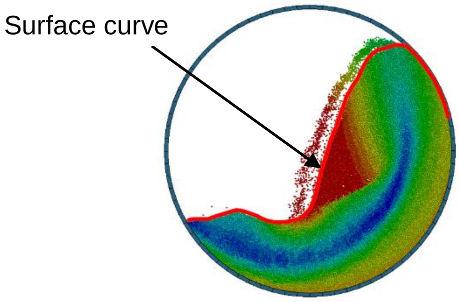

Fig.7: Surface curve of the original (r=1.0 mm) model as target curve of parameter identification

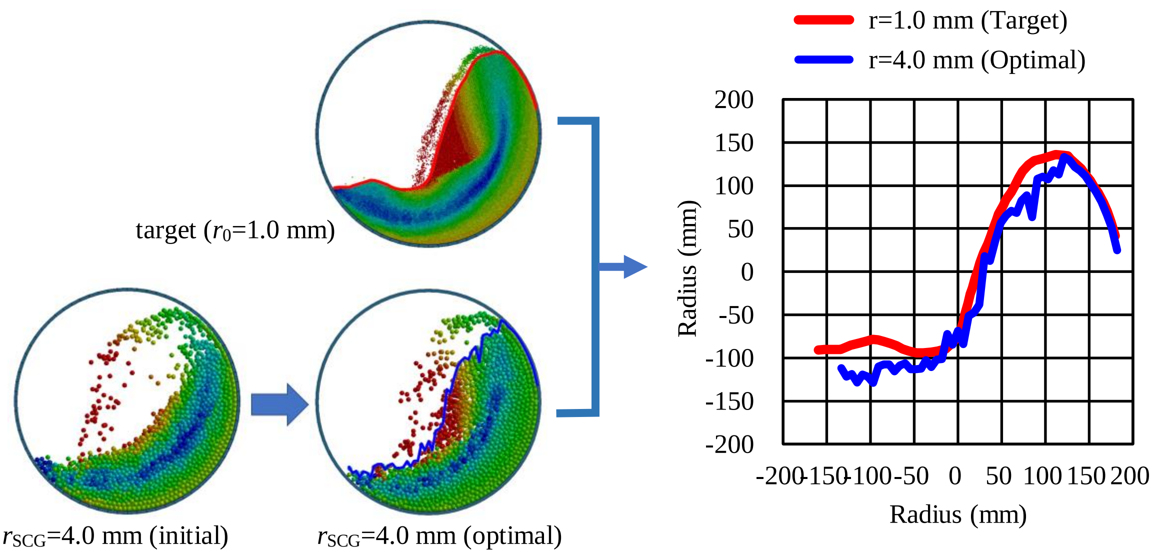

Fig.8: Result of parameter identification for SCG model with r_{SCV}=0.4 mm

Keyword	Variable	Initial value	Optimal value
*CONTROL_DISCRETE_ELEMENT	ndamp	0.5	0.558648808
	tdamp	0.5	0.547304765
	frics	0.3	0.437766112
	fricr	0.1	0.088137162
	normk	0.01	0.095010325
	sheark	0.0029	0.004870718
*DEFINE_DE_TO_SURFACE_COUPLING	frics	0.3	0.398444369
	fricd	0.3	0.186624382
	damp	0.5	0.101806949

Table 3: Parameters used for identification

4 Summary

There are many numerical parameters in DEM model used for modeling machining processes such as conveyance, filling and compression of granular materials. It becomes possible to perform accurate simulation by setting them appropriately. In this paper, parameter identification using optimization software LS-OPT for the compression and rotary drum simulation was reported. In addition, the difference between two coarse graining models were introduced.

5 Literature

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