CALIBRATION OF DISCRETE ELEMENT METHOD SOIL MODELS BASED ON PENETROMETER AND DIRECT SHEAR BOX TESTS USING A GENETIC ALGORITHM

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KEYWORDS

Discrete element method, Soil model calibration, Genetic algorithm, Cone penetration test, Direct shear box test

ABSTRACT

The investigation and mechanical modeling of agricultural soil play an important role in studying the interaction between soil and tillage tools. One of the possible numerical methods for soil modeling is the discrete element method (DEM). Achieving reliable numerical soil-tool interaction studies poses a significant challenge in calibrating various soil models. Calibration of soil models based on physical measurements is feasible. The general aim of calibration is to match as many behavioural mechanical properties of a soil model as possible with the macromechanical properties of the actual soil. Calibration based on physical measurements has previously been an extensive process because during calibration, the micromechanical parameters of the DEM soil model can not be measured directly during physical tests. This research aims to calibrate complex and automated DEM soil model using a genetic algorithms based on penetration and laboratory direct shear box tests. The research results demonstrate that the parameters of the appropriate DEM soil model can be effectively adjusted using genetic algorithms based on the soil's macromechanical properties determined by physical measurements.

ABBREVIATIONS

CPT	Cone Penetration Test
DBST	Direct Shear Box Test
DEM	Discrete Element Method
GA	Genetic Algorithm
PyGAD	Python Genetic Algorithm

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NOMENCLATURE

A_{CP}	Projected area of cone [m^2]
CPR	Cone Penetration Resistance [Pa]
δ	Relative error [%]
f	Fitness value [1]
F_{CP}	Force of cone penetration [N]
F_{Shear}	Shear force [N]
index avg	Average
index k	Normal load variable in DSBTs
index m	Measurement
index s	Simulation

INTRODUCTION

Mechanical soil tillage has played a significant role in agricultural crop production for centuries. The main aims of mechanical soil tillage is to prepare the soil in a condition where crops can grow optimally. The condition of the soil significantly influences crop yield. Proper soil tillage is therefore crucial for sustainable food production. All of this provides reason for intensive research in the numerical modeling of agricultural soils. Some researchers, model soil with the aim of drawing conclusions about soil-tool interactions with minimal physical experimentation. Consequently, tasks related to soil tillage optimization, such as the geometry, arrangement, or parameters of tillage tools, can be performed based on numerical simulations (Aikins et al., 2021). One suitable method for numerical modeling of soil tillage is the discrete element method (DEM). Calibration of various soil models poses the foremost difficulty during numerical simulations, which is feasible based on physical measurements. The aim of this process is to ensure that the macroscopic properties of the numerical granular material model, parametrized with micromechanical characteristics, closely approximate the macroscopic properties of real materials determined during physical measurements. Calibration of soil material has previously been a challenging, slow, and empirical ”trial and error” process, but current research increasingly emphasizes the automatic calibration of DEM models using optimization algorithms. Do et al. 2017 compared the genetic algorithm (GA) with the DIRECT (Jones et al., 1993) optimization technique for setting the micromechanical parameters of quartz sand in DEM. They found that both methods are capable of accurately adjusting the micromechanical parameters of the DEM model with relatively few iterations. They concluded that the application of these methods can reduce calibration costs. The GA is an optimization technique used in unknown search areas, inspired by Darwin's theory of evolution. It evolves the individuals of an initial population over generations (iteratively). In each generation, each individual is tested based on a fitness function, and the characteristics of the best-performing individuals are passed on to the next generation's individuals through parents selection, crossover, and mutation operators. The optimization task can be as completed considered based on various criteria. Do et al. 2018 has introduced a universal framework for the automated calibration of microscopic properties of modeled granular materials. NSGA-II (Non-dominated Sorting Genetic Algorithm II) was employed to solve two material model optimization problems with conflicting objective functions based on a database containing the macroscopic material responses of previous DEM simulations and containing experimental data. Mohajeri et al. 2020 succesfully calibrated the Elasto-Plastic Adhesive DEM model using a Non-dominated Sorting Genetic Algorithm. The macroscopic mechanical properties of carbon powder in DEM were determined based on ring shear test. It is highlighted that the calibration method using the genetic algorithm is independent of the chosen contact model and model parameters. Researchers often employ cone penetration test (CPT) results and laboratory direct shear box test (DSBT) results for calibrating soil models (Kotrocz et al., 2016; Aikins et al., 2023). Safranyik et al. 2017 has already addressed the calibration of DEM soil models using GA based on the results of DBSTs. It was not found any examples in the literature where DEM and GA were applied for the automatic calibration of agricultural soil models based on CPT and DSBT combined test results. The aim of the research is to demonstrate the automatic calibration process of the DEM soil model based on the results of CPT and DSBT conducted on a specific soil.

MATERIALS AND METHODS

Soil measurements

In this study, clay loam soil was subjected to CPT and DSBT, which were used to calibrate a DEM soil model using a genetic algorithm (GA). The soil was previously calibrated based on the same physical measurement results using manual methods by Tamás and Bernon 2021. The penetrometer field tests were conducted at the Hungarian Institute of Agricultural Engineering (NARIC) in Gödöllő, Hungary. Prior to testing, the soil was prepared using a rotary disc harrow to reduce significant surface unevenness caused by clods.

Penetrometer test

During the CPT, the force acting on a conical tool with a projected cross-sectional area of $1cm^2$ was measured as a function of penetration depth according to the NEN 5140:1996 standard. The CPTs were conducted along with soil moisture measurements. In the studied area, tests were performed at 10 arbitrarily selected points to a depth of 800 mm at a speed lower than 20 $mm\,s^{-1}$. The GPS coordinates were recorded for each tested point using the Eijkelkamp penetrometer.

The cone penetration resistance (CPR) was determined by dividing the measured force by the projected area of the cone. Based on the 10 measurements, the average CPR values were determined as a function of depth, along with the soil's average volumetric moisture content, which was found to be 21.3% based on the measurements.

Direct shear box test

The soil samples collected from the field were analyzed at the Soil Mechanics Laboratory of the Budapest University of Technology and Economics (NAT-1-1743/2014). To conduct the DSBT (ISO/TS 17892–2:2004), the moisture content of the samples was adjusted in the laboratory to examine variations in cohesion and internal friction angle for evaluating the DEM models of the soils. The dry based water content was determined using a drying oven (KAPACITÍV KKT. PKL-2002A) at 105°C for 24 hours. During the shear tests, the shear force was measured as a function of relative displacement of the two halves of the 60x60 mm cross-sectional area box up to 6.5 mm displacement. A displacement rate of 0.5 mm/min was applied during the tests, and measurements were conducted under three different normal loads (50 kPa, 100 kPa, 150 kPa) to determine apparent cohesion and friction.

Simulations

For modeling CPT and DSBT, the simulation software based on the Yade-DEM open-source sotware was utilized (Smilauer et al., 2023). To perform automatic soil calibration, a genetic algorithm available in the PyGad library, written for the Python programming environment, was employed (Gad, 2021).

The flowchart illustrating the soil model calibration process using GA is depicted in Figure 1. To run the simulations, a HP Z620 computer with two 20-thread processors was utilized. In order to utilize computer resources more efficiently, simulations were executed in parallel, grouped into generations. Each generation involved testing a total of 38 soil models, with four simulations running for each tested soil model (one of a CPT and three of DSBTs with different normal preloads). The results of the four simulations with identical parameters were collectively evaluated.

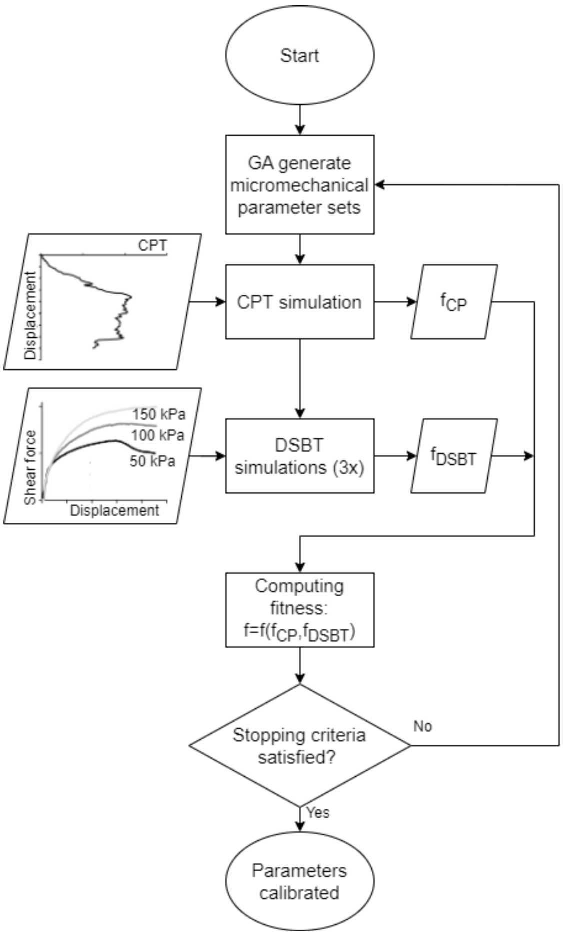

Figure 1: Flowchart of the automated calibration process.

The settings of the GA, which allow the algorithm to generate individuals performing better based on the previous generation, by apply parents selection, crossover, and mutation operators, are provided in Table 1.

Table 1: The settings of the GA.

Name of parameter	Value of parameter
Number of solutions per population	38
Number of generation	10
Number of parents mating	8
Number of genes	4
Mutation percent of genes [%]	1.5

Simulation environments were developed separately for both CPT and DSBT modeling as shown in Figure 2. In both simulations, the arrangement of measurements and geometric conditions were modeled to correspond to real physical measurements. For CPT modeling, a 140x140 mm cross-sectional area, 300 mm high box was created, into which the elements were settled gravitationally. After settling, the surface of the assembly was cut, and a penetrometer with a projected cross-sectional area of 250 mm^2 was placed 4.5 mm above the top element, in the center of the box, and uniformly pushed into the assembly at a speed of 0.5 $m\,s^{-1}$. In the simulated DSBT, a box with a cross-sectional area of 60x60 mm was created. The height of the bottom part was 15 mm, and the height of the top part was 240 mm. The granular assembly was deposited gravitationally in this box. After depositing, the surface of the assembly was cut at a height of 45 mm from the bottom of the lower box, and then an utilsbox element was released onto the top of the assembly. This element provided the normal preload, with only the vertical degree of freedom was allowed. The dimensions of the utilsbox were tailored to the cross-sectional area of the shear box, with a height of 20 mm determined for this purpose. The density of the material of the utilsbox used to define the preload was determined such that it exerted a normal pressure on the assembly consistent with physical measurements.

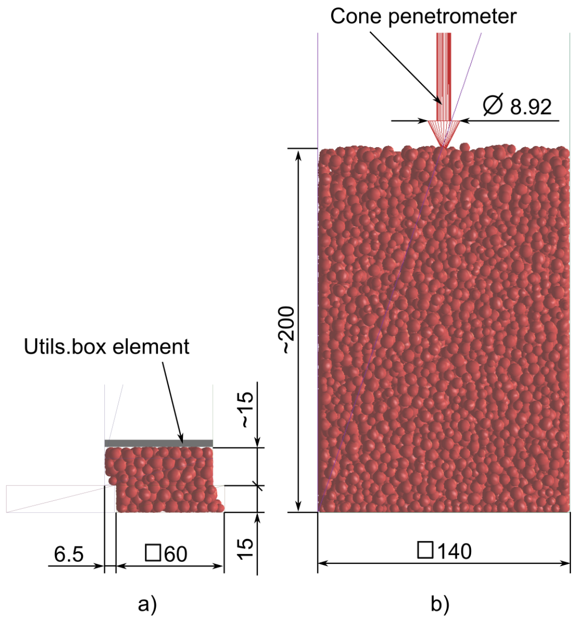

Figure 2: The arrangement of the a) DSBT and b) CPT simulations. (Dimensions are in mm.)

In the simulations, quantities measured during physical experiments were recorded. In the simulated CPT, the soil resistance acting on the cone was plotted as a function of penetration depth. In the DSBT, the summed forces acting on the lower part of the box were recorded as a function of displacement. The DSBT simulations were conducted with three different preloads (50 kPa, 100 kPa, 150 kPa), consistent with the physical measurements.

The calibration aim is to simultaneously approach with as much accuracy as possible the values of quantity pairs recorded during the physical measurements in both CPT and DSBT simulations using identical sets of relationship parameter settings. This necessitates evaluating the soil models tested in each simulation individually, and then collectively across simulations with identical relationship parameter settings. It is important to employ an objective evaluation system that equally weighs the results of the CPT and the three DSBT simulations.

The results of each simulations were compared with the results of the physical measurements. In the case of CPT, relative errors were calculated for average CPR values obtained from physical measurements and simulated CPR values at equivalent depths, and the average of these errors was taken according to Equation 2.

$$CPR = \frac{F_{CP}}{A_{CP}} \tag{1}$$

$$\bar{\delta}_{CPR} = \frac{1}{n} \cdot \sum_{i=1}^{n} \frac{|CPR_{s,i} - CPR_{m,i}|}{CPR_{m,i}} \cdot 100 \tag{2}$$

In the case of DSBT, relative errors were calculated for shear force values obtained from physical measurements and simulated shear force values at equivalent displacements of the shear box, and the average of these errors was taken according to Equation 3.

$$\bar{\delta}_{F_{Shear}} = \frac{1}{n} \cdot \sum_{i=1}^{n} \frac{|F_{Shear,s,i} - F_{Shear,m,i}|}{F_{Shear,m,i}} \cdot 100 \tag{3}$$

The results of each simulation were evaluated with a number between 0 and 1. The higher the value assigned to a simulation, the closer the result was found to the physical measurements. In the case of CPT, to the calculations, the relative error values were based on, according to Equation 4.

$$f_{CPT} = 1 - \frac{\bar{\delta}_{CPR}}{100} \tag{4}$$

Since three DSBT simulations were conducted with identical parameters but different normal loads, the results of the DSBT simulations were aggregated with a weight of 1/3 each. In Equation 5, the index k refers to the different normal loading cases.

$$f_{DSBT,k} = 1 - \frac{\bar{\delta}_{F_{Shear}}}{100} \tag{5}$$

$$f_{DSBT} = \frac{1}{3} \cdot \sum_{k=1}^{3} f_{DSBT,k} \tag{6}$$

If the value of $f_{DSBT,k}$ or f_{CPT} would take a negative value, it is replaced by 0.

The results of the CPT and DSBT tests were aggregated according to Equation 9. This function represents the fitness function of the genetic algorithm. In defining this function, efforts were made to reward combinations with identical input parameters f_{CPT} and f_{DSBT} more, and if either f_{CPT} or f_{DSBT} is 0, the result should be 0.

$$f_a = sin\left(f_{CPT} \cdot \frac{\pi}{2}\right) \cdot sin\left(f_{DSBT} \cdot \frac{\pi}{2}\right) \tag{7}$$

$$f_b = (f_{CPT} \cdot f_{DSBT}) + (1 - f_{CPT}) \cdot (1 - f_{DSBT}) \tag{8}$$

$$f = f_a \cdot f_b \tag{9}$$

A basic set of simulation settings and genetic algorithm (GA) settings for calibrating the micromechanical parameters of the soil model are provided in Table 2. It also includes the four genes and value intervals of the soil model.

Table 2: Simulation settings and contact parameters of the modelled materials. The table includes also the four genes and value intervals of the soil model as variable parameters.

Name of parameter	Value of parameter
Element type	sphere
Micromechanical Young's Modulus of soil model [Pa]	variable (10^6 - 10^7)
Rolling and twisting friction coefficient [1]	variable (0.001 - 0.4)
Friction angle [°]	variable (10 - 40)
Normal cohesion [Pa]	variable (0 - 10^6)
Shear cohesion [Pa]	0.5·Normal cohesion
Density [$kg\, m^{-3}$]	2700
Micromechanical Poisson-coefficient [1]	0.4
Radius of sphere element and uniform radius distribution [m]	$0.003 \pm 30\%$,
Global damping during deposition [1]	0.8
Global damping during simulated measurements [1]	0
Density of wall and tool elements [$kg\, m^{-3}$]	7850
Young's Modulus of wall and tool elements [Pa]	10^9
Micromechanical Poisson-coefficient of wall and tool elements [1]	0.3
Friction angle of wall and tool elements [°]	40
Timestep during deposition [s]	0.5·Rayleigh's estimated static time step
Timestep during simulated measurements [s]	0.1·Rayleigh's estimated static time step
Initial unbalanced force [1]	0.02
Speed of penetrometer [$m\, s^{-1}$]	0.5
Speed of DSBT [$m\, s^{-1}$]	0.05

RESULTS AND DISCUSSION

The automated DEM soil model calibration process based on CPT and DSBT physical measurements using GA appears promising, although adjustments in the simulations need to be further refined to achieve better results. Next, the results of the simulations will be discussed. During the simulation studies, 408 CPT and 3x408 DBST were examined with the contact parameter combinations generated by GA, as shown in Tables 1 and 2. Running all simulations with the presented settings took 46 hours.

Results of CPT Simulations

Analyzing the results of the CPT simulations independently of the DSBT results, it was observed that up to a depth of 0.15 m, the $\bar{\delta}_{CPR}$ value was 40% in the best case scenario. This value is quite high, indicating that even in the best results, the simulated curve can only follow the measured curve up to a depth of 0.1 m. Below 0.1 m depth, CPR values do not increase further, lagging behind the measured values. This confirms the suggestion by Tamás and Bernon (2021) to create multiple soil model layers with different sets of micromechanical parameters in simulations.

Results of DSBT Simulations

Analyzing the results of the DSBT simulations independently of the CPT results, it was observed that for normal stresses of 50 kPa, 100 kPa, and 150 kPa, the best-case $\bar{\delta}FShear, k$ values were 8%, 16%, and 30%, respectively. From this, it was concluded that as the normal preload increases, the simulated curves are better able to approximate the measured curves. However, it is important to note that while a high level of agreement is observed in the tests with a preload of 150 kPa, tests with preloads of 100 kPa and 50 kPa result in higher errors. An example of this is the following case. The best combined result obtained according to Equation 10 during DSBT simulations was 22%. In this case, for preloads of 50 kPa, 100 kPa, and 150 kPa, the $\bar{\delta}FShear, k$ values were 8%, 27%, and 36%, respectively.

$$\bar{\delta}_{F_{Shear},avg} = \frac{1}{3} \cdot \sum_{k=1}^{3} \bar{\delta}_{DSBT,k} \tag{10}$$

It was also noted that in the best DSBT results, the simulated curves typically approached the measured curves from below.

Combined CPT and DSBT results

The soil model with the micromechanical parameters listed in Table 3 achieved the best approximation of simultaneously DSBT and CPT physical measurement results. In this case, the $\bar{\delta}FShear, avg$ value was 27%, and the $\bar{\delta}_{CPR}$ value was 41%.

Table 3: The contact parameters of the modeled clay loam soil in the case of the best result.

Name of parameter	Value of parameter
Micromechanical Young's Modulus of soil model [Pa]	$8.809 \cdot 10^6$
Rolling and twisting friction coefficient [1]	0.1279
Friction angle [°]	18.85
Normal cohesion [Pa]	$2.770 \cdot 10^5$

The results of the simulations conducted on the soil model described by the parameters in Table 3 are shown in Figure 3.

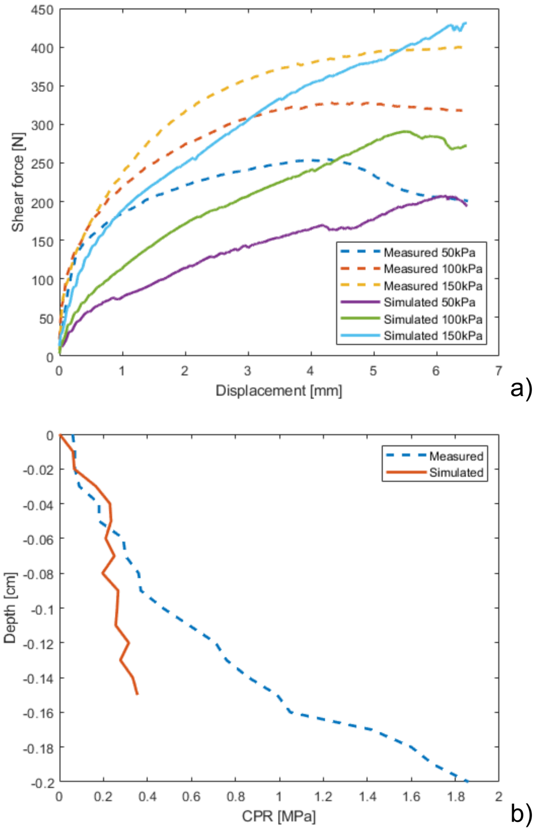

Figure 3: The best result of automatic soil calibration during the a) DSBTs and b) CPTs, utilizing the most suitable soil model identified by the GA.

In Figure 4, using the ParaView software (Ahrens et al., 2005), the velocities of the elements and the normal forces between the elements were visualized in the simulation of DSBTs (a) and CPTs (b). The soil model was configured with the parameters listed in Table 3 also for visualization.

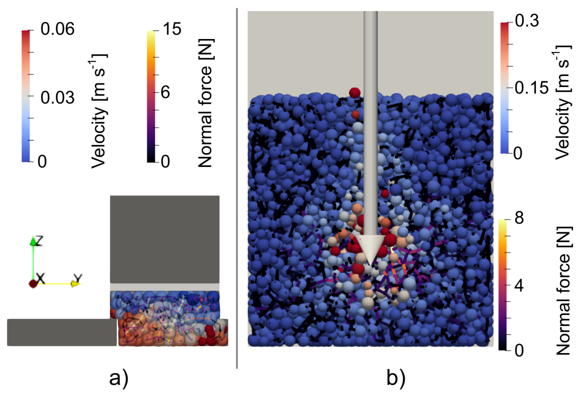

Figure 4: The velocities of the elements and the normal forces between the elements have been visualized in the simulation results of a) DSBTs and b) CPTs.

CONCLUSIONS

In this study, a method was developed for automatically calibrating DEM soil models using a genetic algorithm based on physical CPT and DSBT measurement results. The calibration aim is to find micromechanical parameter combinations characteristic of a DEM soil model, such that conducting CPTs and DSBTs with these parameters yields results similar to the measured ones. An objective evaluation method was established that equally considered the simulation results of CPT and DSBT tests compared to the physical measurements. Throughout the research, the following conclusions were drawn:

- The automatic calibration process proved to be effective, with the GA finding better solutions as generations progressed.
- During simulations, CPR values could only be described with identical micromechanical parameter combinations up to a depth of 0.1 m.
- In DSBT tests, the measured values are typically approached from below by the best simulated solutions.
- In the best-case scenario, the $\bar{\delta}_{FShear,avg}$ value was 27%, and the $\bar{\delta}_{CPR}$ value was 41%.

FURTHER TASKS

In the future, the following suggestions have been proposed to refine the soil model:

- Since the variation of CPR values differs from the variation of F_{Shear} in physical measurements, it is recommended to take this into account when calculating the fitness value by considering the ratio of dispersions.
- It is suggested to run additional generations beyond 10.
- It is recommended to experiment with the application of DEM models with additional contact parameters (such as eg. damping) (Horváth et al., 2019).

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