

Analysis and Improvement of the  
Time-Driven Discrete Element Method

Dissertation  
zur  
Erlangung des Grades  
Doktor-Ingenieur  
der  
Fakultät für Maschinenbau  
der Ruhr-Universität Bochum

von

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aus Herne

Bochum 2007

Dissertation eingereicht am: 10.09.07  
Tag der mündlichen Prüfung: 16.11.07

Erster Referent: Prof. Dr.-Ing. V. Scherer  
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Berichte aus der Energietechnik

**Harald Kruggel-Emden**

**Analysis and Improvement of the Time-Driven  
Discrete Element Method**

Shaker Verlag  
Aachen 2008

**Bibliografische Information der Deutschen Nationalbibliothek**

Die Deutsche Nationalbibliothek verzeichnet diese Publikation in der Deutschen Nationalbibliografie; detaillierte bibliografische Daten sind im Internet über <http://dnb.d-nb.de> abrufbar.

Zugl.: Bochum, Univ., Diss., 2007

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Printed in Germany.

ISBN 978-3-8322-6853-4  
ISSN 0945-0726

Shaker Verlag GmbH • Postfach 101818 • 52018 Aachen  
Telefon: 02407 / 95 96 - 0 • Telefax: 02407 / 95 96 - 9  
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## **Vorwort**

Die vorliegende Arbeit entstand am Lehrstuhl für Energieanlagen und Energieprozesstechnik der Ruhr-Universität Bochum im Rahmen eines Promotionsstipendiums. An dieser Stelle ist daher ausdrücklich dem Allgemeinen Promotionskollegs der Ruhr-Universität Bochum und der Studienstiftung des Deutschen Volkes für die finanzielle aber auch weitreichende ideelle Förderung zu danken. Zudem wurde durch den Lehrstuhl die Aufstockung des Stipendiums durch eine Mitarbeiterzeitstelle ermöglicht.

An dieser Stelle möchte ich ebenfalls all denjenigen meinen Dank aussprechen, die mich bei der Ausarbeitung und Fertigstellung dieser Arbeit unterstützt haben. In besonderer Weise möchte ich Herrn Prof. Dr.-Ing. Viktor Scherer für die Möglichkeit danken, diese Arbeit unter seiner wissenschaftlichen Leitung durchzuführen und dann auch das Hauptreferat zu übernehmen. In diesem Zusammenhang hat gerade die gewährte wissenschaftliche Freiheit entscheidend zum Gelingen dieses Promotionsvorhabens beigetragen.

Gleichfalls danke ich Junior-Prof. Dr.-Ing. Marcus Petermann für die freundliche Übernahme des Korreferates.

Herrn Dr.-Ing. Siegmar Wirtz gebührt Anerkennung für seine Betreuung und durchgehende Unterstützung. Insbesondere der Wissensaustausch und die kritische Diskussion erzielter Ergebnisse waren hilfreich.

Mein Dank gilt zudem meinen direkten Kollegen des Lehrstuhls, aber auch denen anderer Lehrstühle der Fakultäten für Maschinenbau und Bauingenieurwesen, und zwar für die freundliche kollegiale Atmosphäre, durch die ein harmonisches und effektives Arbeitsklima geschaffen wurde. Besonders danke ich Frau Mira Sturm, Herrn Peter Knüpfer, Herrn Sven Langbein, Herrn Patrick Luig, Herrn Stefan Rickelt, Herrn Lars Röchter und Herrn Erdem Simsek unter anderem für die kritische Durchsicht des Manuskripts und die vielen offenen Diskussionen, aus denen sich wertvolle Anregungen für diese Arbeit ergeben haben. Dank sage ich gleichfalls meinen Mitstipendiaten des Promotionskollegs, und denen der Studienstiftung des Deutschen Volkes für die vielen anregenden Gespräche und die interessanten Einblicke in andere Fachbereiche, die während der zahlreichen Treffen zustande kamen.

Meiner Familie, insbesondere meinen Eltern, und meinen Freunden danke ich für die herzliche Unterstützung, auf die ich mich bei der Entstehung dieser Arbeit immer verlassen konnte.



## **Abstract of the Dissertation**

Several processes in nature as well as many industrial applications involve static or dynamic granular materials. Granulates can adopt solid, liquid or gas like states and thereby reveal intriguing physical phenomena not observable in its versatility for any other form of matter. The frequent occurrence of phase transitions and the related characteristics thereby strongly affect their processing quality and economics. This situation demands for prediction methods for the behavior of granulates. In this context simulations provide a feasible alternative to experimental investigations. Advantageous are their better reproducibility, their less expenditure of time and their lower costs. Several different simulation approaches are applicable to granular materials. The time-driven Discrete Element Method turns out to be the most complex but also as the most general method. It is based on tracking each particle's movement and its interactions with the surrounding over time. The method provides detailed information on particle positions, orientations and translational and angular velocities. These properties are obtained by integrating numerically a set of fully deterministic differential equations which are explicitly depending on the contact forces.

The time-driven Discrete Element Method is a simulation approach which has been used in a wide variety of scientific fields for more than thirty years. With the tremendous increase in available computer power, especially in the last years, the method is more and more developing to the state of the art simulation technique for granular materials. Despite of the long time of usage, model advances and theoretical and experimental studies are not harmonized in the different branches of application, providing a large potential for improvements.

Therefore, the scope of this work is a review of methods and models based on theoretical considerations and experimental data from literature. Through model advances it is intended to contribute to a general enhancement of techniques, which are then directly available for simulations.

In detail, force displacement models which are usually separated in normal and tangential direction are reviewed for a broad range of experimental data. Model improvements and new methods for the derivation of simulation parameters are proposed. For a special combination of force models an analytical solution is derived, which is later used as a benchmark case for the evaluation of different integration schemes. With the Discrete Element Method even today being mostly limited to simple spherical bodies a method for the implementation of complex shapes based on multi-sphere particles is reviewed. The applicability of this approach is verified based on a study on collision properties under different impact situations. As a final application outlining the advantages of particle orientated modeling the Discrete Element Method incorporating the derived improvements is used for a comparative study of mixing on grates.



**Contents**

1. Introduction .....	1
1.1. Physical Phenomena .....	1
1.2. Industrial Relevance of Granular Materials .....	3
1.3. Modeling of Particle Systems .....	4
1.3.1. Event-Driven Discrete Element Method.....	5
1.3.2. Direct Simulation Monte Carlo Method.....	7
1.3.3. Time-Driven Discrete Element Method.....	7
1.4. Research Demand and Objectives.....	10
2. Review and Extension of Normal Force Models .....	13
2.1. Quantities Accessible during Impact .....	14
2.2. Considered Normal Force Models .....	17
2.2.1. Continuous Potential Models .....	18
2.2.2. Linear Viscoelastic Models .....	19
2.2.3. Non-Linear Viscoelastic Models .....	20
2.2.4. Hysteretic Models .....	22
2.3. Determination of the Coefficients of the Models .....	26
2.3.1. Outline of the Adjustment Procedure.....	26
2.3.2. Calculated Model Coefficients .....	28
2.4. Discussion of Models .....	31
2.5. Comparison of Models with Experimental Data .....	32
2.6. Extension of the Classical Models .....	36
2.6.1. Extension of the Linear Models .....	37
2.6.2. Extension of the Non-Linear Viscoelastic Models.....	40
2.7. Comparison of Extended Models to Experimental Data.....	41
3. Review of Tangential Force Laws.....	45
3.1. Quantities Accessible during Impact .....	45
3.2. Comparison of Force Models .....	47
3.2.1. Normal Force Models Employed .....	47
3.2.2. Tangential Force Models Considered.....	48
3.2.2.1. Linear Tangential Models.....	48
3.2.2.2. Non-Linear Tangential Models .....	52
3.3. Determination of the Model Parameters.....	55
3.3.1. Model Parameters in Normal Direction.....	55
3.3.2. Model Parameters in Tangential Direction.....	57
3.4. Comparison of Experimental Results with Simulations .....	60
3.4.1. Experiments with Constant Coefficient of Normal Restitution.....	61
3.4.1.1. Influence of Normal Force Models .....	61
3.4.1.2. Performance of Tangential Models .....	61
3.4.2. Experiments with Varying Coefficient of Normal Restitution .....	63
3.4.2.1. Influence of Normal Force Models .....	63
3.4.2.2. Performance of Tangential Models .....	65
4. Derivation of an Analytical Contact Model Solution .....	73

4.1. Equations of Motion .....	73
4.1.1. Solution in Normal Direction .....	76
4.1.2. Solution in Tangential Direction for the Contact Point .....	76
4.1.3. Solution in Tangential Direction for the Center of Mass .....	78
4.2. Model Parameters .....	79
4.3. Detailed Analysis of the Collision Modes .....	80
4.3.1. Small Impact Angles .....	83
4.3.2. Intermediate Impact Angles .....	83
4.3.3. Large Impact Angles .....	85
4.4. Computational Implementation .....	85
4.5. Comparison of Analytical with Experimental and Numerical Data .....	86
5. Review of Explicit Time Integration Schemes .....	91
5.1. Considered Numerical Schemes .....	92
5.1.1. One Step Algorithms .....	92
5.1.2. Multi Step Algorithms .....	95
5.1.3. Predictor-Corrector Algorithms .....	97
5.2. Comparison of the Algorithms .....	99
5.2.1. Integration Accuracy .....	100
5.2.2. Time Grid Accuracy .....	104
5.2.3. CPU-Requirements .....	106
5.2.4. Computational Efficiency .....	107
6. Modeling of Complex Shapes .....	115
6.1. Brief Overview of Methods .....	115
6.2. Multi-Sphere Method .....	118
6.2.1. Equations of Motion .....	119
6.2.2. Integration of Translation and Rotation .....	120
6.2.3. Calculation of Contact Forces .....	121
6.3. Method Evaluation for Specific Collision Setups .....	123
6.3.1. Multiple Contact Collisions .....	125
6.3.2. Single Contact Collisions .....	126
7. DEM Application: A Study of Particle Mixing on Grates .....	131
7.1. Simulation Setting .....	131
7.2. Mixing Properties .....	132
7.2.1. Velocity Based Approach .....	132
7.2.2. Trajectory Based Approach .....	134
7.3. Determination of Simulation Parameters .....	135
7.4. Results .....	137
7.4.1. Forward Acting Grate in 2D .....	138
7.4.2. Forward Acting Grate in 3D .....	140
7.5. General Comparisons .....	141
8. Summary and Prospect .....	143
9. Bibliography .....	149

## Glossary

### Latin Glossary:

Variable	Unit	Denotation
$a$	$[m/s^2]$	acceleration
$A$	$[1/m]$	normal force model parameter
$A$	$[ - ]$	tangential force model parameter
$b$	$[m/s^3]$	first time derivative of the acceleration
$B$	$[ - ]$	tangential force model parameter
$c$	$[ - ]$	dimensionless exponent
$c$	$[m/s^4]$	second time derivative of the acceleration
$C$	$[ - ]$	tangential force model parameter
$d$	$[m]$	diameter
$D$	$[ - ]$	tangential force model parameter
$D$	$[m]$	normalized particle depth
$\bar{D}$	$[m]$	mean normalized particle depth
$\tilde{D}$	$[m]$	fluctuating normalized particle depth
$e$	$[ - ]$	coefficient of restitution
$E$	$[kg/(m s^2)]$	Young's modulus
$\vec{E}$	$[ - ]$	unit vectors in the inertial frame
$\vec{E}$	$[ - ]$	unit vectors in the body fixed frame
$\vec{F}$	$[kg m/s^2]$	force vector
$g$	$[m/s^2]$	acceleration of gravity
$\bar{g}$	$[m/s^2]$	acceleration of gravity vector
$G$	$[kg/(m s^2)]$	shear modulus
$h$	$[m]$	height
$h_r$	$[m/s]$	position related integration scheme parameter
$h_v$	$[m/s^2]$	velocity related integration scheme parameter
$i$	$[ - ]$	integral indices
$I$	$[ - ]$	integral indices
$I$	$[kg m^2]$	inertia tensor
$\hat{I}$	$[kg m^2]$	inertia tensor along principal axis
$j$	$[ - ]$	integral indices
$J$	$[ - ]$	integral indices
$k$	$[ - ]$	integral indices
$k$	$[kg/s^2]$	linear stiffness
$\tilde{k}$	$[kg/(m^{1/2}s^2)]$	non-linear stiffness
$K$	$[ - ]$	integral indices
$l$	$[ - ]$	integral indices
$l$	$[m]$	length

$L$	$[ - ]$	integral indices
$L$	$[m]$	length
$\Delta l$	$[m]$	amplitude
$m$	$[kg]$	mass
$m$	$[ - ]$	integral indices
$M$	$[ - ]$	integral indices
$\vec{M}$	$[kg\ m^2 / s^2]$	moment vector
$n$	$[ - ]$	set of coefficients
$n$	$[ - ]$	integral indices
$\vec{n}$	$[ - ]$	normal vector
$N$	$[ - ]$	integral indices
$o$	$[ - ]$	integral indices
$O$	$[ - ]$	error order
$O$	$[ - ]$	integral indices
$p$	$[ - ]$	normal force model parameter
$p_y, \tilde{p}_y$	$[N/m^2]$	materials yield point
$\tilde{p}$	$[m/s]$	standard deviation of fluctuating velocities
$p$	$[m/s]$	scalar standard deviation of fluctuating velocities
$\vec{P}'$	$[m/s]$	velocity based mixing property
$P'$	$[m/s]$	scalar velocity based mixing property
$\Delta \vec{P}$	$[kg\ m/s]$	change of momentum
$q$	$[ - ]$	normal force model parameter
$Q'$	$[m/s]$	position based time averaged mixing property
$r$	$[m]$	radius
$r$	$[ - ]$	non-dimensional radius
$r$	$[m]$	position
$r_v$	$[m]$	evaluation radius
$R$	$[m]$	radius
$s$	$[1/m]$	normal force model parameter
$s$	$[m]$	coordinate of the contact point
$t$	$[s]$	time
$t'$	$[s]$	time
$\Delta t$	$[s]$	time step
$\vec{t}$	$[ - ]$	tangential vector
$t^n$	$[s]$	duration of a collision
$v$	$[m/s]$	velocity
$v_{00}$	$[(m/s)^{\chi_2}]$	normal force model parameter
$\vec{v}$	$[m/s]$	velocity vector
$\tilde{\vec{v}}$	$[m/s]$	mean velocity vector
$\tilde{\tilde{v}}$	$[m/s]$	fluctuating velocity vector
$w$	$[ - ]$	weighting factor

$W$	$[m]$	grate width
$\vec{W}$	$[1/s]$	angular velocity vector
$\vec{x}$	$[m]$	position vector
$x$	$[m]$	Cartesian coordinates
$x$	[varying]	independent variable
$X$	$[m]$	distance between particle centers
$y$	[varying]	dependent variable
$y$	$[m]$	Cartesian coordinates
$z$	$[m]$	Cartesian coordinates

**Greek Glossary:**

Variable	Unit	Denotation
$\alpha$	$[rad]$	collision angle
$\alpha$	$[rad]$	grate declination
$\alpha_l$	$[kg\ m^{1-p} / s^2]$	empirical material stiffness during loading
$\alpha_{ul}$	$[kg\ m^{1-p-q} / s^2]$	empirical material stiffness during unloading
$\beta^n$	$[-]$	damping ratio
$\beta_1$	$[-]$	sliding coefficient of tangential restitution
$\beta_0$	$[-]$	sticking coefficient of tangential restitution
$\beta$	$[-]$	effective coefficient of tangential restitution
$\beta$	$[rad]$	rebound angle
$\beta$	$[rad]$	grate inclination
$\gamma$	$[kg/s]$	velocity proportional damping coefficient
$\hat{\gamma}$	$[kg/(s\ m^{1/4})]$	non-linear damping coefficient
$\bar{\gamma}, \hat{\gamma}$	$[1/s]$	dissipation coefficient
$\tilde{\gamma}$	$[kg/(s\ m^{1/2})]$	non-linear damping coefficient
$\check{\gamma}$	$[kg/(s\ m^{\tilde{\Theta}})]$	non-linear damping coefficient
$\delta$	$[1/s]$	frequency
$\delta$	$[m]$	overlap or normal displacement
$\delta^v, \delta^{\Delta x}, \delta^x, \delta^d$	$[-]$	binary condition functions
$\varepsilon^n$	$[kg\ m^2/s^2]$	characteristic energy
$\varepsilon$	$[-]$	integration method parameter
$\varepsilon$	$[rad]$	tilting angle
$\eta$	$[-]$	material property
$\tilde{\Theta}$	$[-]$	dimensionless exponent
$\theta$	$s^\eta/m^\eta$	material property
$\theta$	$[rad]$	angle of revolution
$\dot{\theta}$	$[1/s]$	angular velocity
$\iota$	$[rad]$	tilting angle
$\kappa$	$[-]$	tangential to normal stiffness ratio
$\Lambda$	$[-]$	rotation matrix

$\Delta\Lambda$	[–]	incremental rotation matrix
$\mu$	[–]	friction coefficient
$\nu$	[–]	Poisson's ratio
$\xi$	[m]	overlap or normal displacement
$\xi'$	[m]	elongation of the spring in tangential direction
$\vec{\xi}'$	[m]	elongation vector of the tangential spring
$\dot{\xi}$	[m/s]	normal displacement rate
$\ddot{\xi}$	[m/s <sup>2</sup> ]	normal acceleration
$\xi_f$	[m]	final resulting displacement
$\xi_r$	[–]	displacement ratio
$\xi_y$	[m]	displacement at yield point
$\dot{\xi}_y$	[m/s]	displacement rate at yield point
$\xi_0'$	[m]	micro structural surface roughness
O	[–]	Heaviside function
$\tilde{\pi}$	[kg m <sup>2</sup> / s]	angular momentum
$\rho$	[kg/m <sup>3</sup> ]	density
$\varsigma$	[–]	functional relation
$\phi$	[kg m <sup>2</sup> /s <sup>2</sup> ]	continuous potential
$\phi$	[varying]	measurable quantity
$\bar{\phi}$	[rad]	angle of revolution
$\chi_1$	[(m/s) <sup><math>\chi_2</math></sup> ]	normal force model parameter
$\chi_2, \chi_4$	[–]	normal force model parameter
$\chi_3$	[m <sup><math>\chi_4</math></sup> · s <sup>1-<math>\chi_4</math></sup> ]	normal force model parameter
$\chi^2$	[varying]	weighted sum of squares
$\vec{\psi}$	[–]	vectorial rotation angle
$\psi$	[–]	normal force model parameter
$\psi_1$	[–]	dimensionless initial tangential velocity
$\psi_2$	[–]	dimensionless final tangential velocity
$\omega$	[1/s]	frequency
$\omega$	[1/s]	angular velocity
$\vec{\omega}$	[1/s]	angular velocity vector

### Subscripts:

Variable	Denotation
0	initial
<i>analy</i>	analytical
<i>bot</i>	bottom
<i>c</i>	critical
<i>CG</i>	center of gravity
<i>eff</i>	effective
<i>el</i>	elastic

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<i>exp</i>	experimental
<i>diss</i>	dissipative
<i>f</i>	final
<i>F0</i>	at zero force
<i>i</i>	integer indices
<i>j</i>	integer indices
<i>k</i>	integer indices
<i>l</i>	loading
<i>m</i>	mean
<i>max</i>	maximal
<i>min</i>	minimal
<i>mod</i>	model
<i>num</i>	numerical
<i>nonel</i>	non-elastic
<i>p</i>	predicted
<i>PP</i>	particle/particle
<i>pt</i>	potential derived
<i>PW</i>	particle/wall
<i>rl</i>	reloading
<i>s</i>	relative to the contact point
$t \pm n \cdot \Delta t$	at time $t \pm n \cdot \Delta t$
<i>top</i>	top
<i>ul</i>	unloading
<i>x</i>	relative to the <i>x</i> -axis
<i>y</i>	relative to the <i>y</i> -axis
<i>z</i>	relative to the <i>z</i> -axis

**Superscripts:**


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Variable	Denotation
$-1$	inverse
$'$	final collision quantity
$*$	state of reversion
$n$	normal direction
$t$	tangential direction
$T$	transposed