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chemengineering Article A Coarse Grained Model for Viscoelastic Solids in Discrete Multiphysics Simulations Iwan H. Sahputra 1,2,* , Alessio Alexiadis 1 and Michael J. Adams 1 1 School of Chemical Engineering, University of Birmingham, Birmingham B15 2TT, UK; a.alexiadis@bham.ac.uk (A.A.); m.j.adams@bham.ac.uk (M.J.A.) 2 Industrial Engineering Department, Petra Christian University, Surabaya 60236, Indonesia * Correspondence: iwanh@petra.ac.id ?????????? Received: 10 March 2020; Accepted: 25 April 2020; Published: 1 May 2020 ??????? Abstract: Viscoelastic bonds intended for Discrete Multiphysics (DMP) models are developed to allow the study of viscoelastic particles with arbitrary shape and mechanical inhomogeneity that are relevant to the pharmaceutical sector and that have not been addressed by the Discrete Element Method (DEM). The model is applied to encapsulate particles with a soft outer shell due, for example, to the partial ingress of moisture. This was validated by the simulation of spherical homogeneous linear elastic and viscoelastic particles. The method is based on forming a particle from an assembly of beads connected by springs or springs and dashpots that allow the sub-surface stress fields to be computed, and hence an accurate description of the gross deformation. It is computationally more expensive than DEM, but could be used to define more effective interaction laws. Keywords: Kelvin–Voigt viscoelastic bonds; coarse grained model; particle method; viscoelastic particles; inhomogeneous particles 1. Introduction The Discrete Element Method (DEM) has been employed to study a range of pharmaceutical manufacturing processes and products including powder mixing [1], agglomeration with and without a liquid binder [2], and the release of Active Pharmaceutical Ingredients (APIs) from powder inhalation products [3]. Invariably, this has not involved inhomogeneous particles, and those of arbitrary shape have been simulated by gluing primary particles together such that the interior is essentially rigid in order to minimise the computational cost, which is not representative of real particles [4]. An important example of mechanical inhomogeneity is the softening of particles due the presence of moisture during agglomeration or dispersion/dissolution. In such cases, a gradient of moisture content is developed with a corresponding gradient in the mechanical properties. Another example is the encapsulation of APIs for which there is commonly a hard shell and a softer core. For particles formed from an organic polymer such as microcrystalline cellulose, the ingress of moisture will cause them to become viscoelastic. Mesh-free methods and, in particular, particle methods such as DEM are increasingly popular in the scientific community due to their ability to overcome some drawbacks of the conventional, mesh-based, numerical methods; see [5] for a review. Particle methods can also be coupled together within a Discrete Multiphysics (DMP) framework that, unlike conventional multiphysics techniques, is based on “computational particles” rather than on computational meshes [6,7]. In fact, there is a range of systems for which DMP can address problems that would be very difficult, if not impossible, for traditional multiphysics approaches. Examples are cardiovascular valves [8,9], blood clotting [10], phase transitions [11], capsules’ breakup [12,13], and fuzzy boundaries (e.g., a tablets’ dissolution) [14]. In many of the above examples, the solid phase is often represented by a Lattice Spring Model (LMS) ChemEngineering 2020, 4, 30; doi:10.3390/ chemengineering4020030 www.mdpi.com/journal/chemengineering and involves both linear and non-linear springs for modelling elastic materials. In the current study, the method is extended to viscoelastic materials by implementing the Kelvin–Voigt (KV) viscoelastic model that involves springs and also dashpots to represent the viscous friction. KV bonds have been proposed in the LSM literature, but only to model wave propagation in viscoelastic media (e.g., seismic wave propagation [15]), where the media are treated as homogenous and no external forces are applied to the system. KV bonds have never been implemented to study the strain field of solid objects under the effect of external loads. Achieving this objective would provide particle-based multiphysics techniques (e.g., DMP) with the ability to model viscoelastic materials, which is currently not possible. The current study addresses the above shortcoming in the literature. For benchmark and validation purposes, the diametric compression of homogeneous spherical particles between parallel platens is described, which may be considered as a special case of indentation. A flat indenter or platen is widely used especially for the diametric compression of single particles [16] and microcapsules [17]. Generally, they are loaded at a constant velocity to a specified displacement and unloaded, or alternatively held in position, to measure the stress relaxation. A quasistatic model based on Hertz’s contact theory has been employed to describe the interaction between the particles that are packed together to represent unconsolidated porous media [18]. The evolution of the permeability with the deformation was computed by the lattice-Boltzmann approach. Here, the approach is that macroscopic bodies (such as particles) are sub-divided into computational beads. Each bead is connected to the nearest neighbours by linear springs or by KV bonds. It will be shown that for the spherical particle represented by beads connected by linear springs model, under diametric compression simulation, the relationship between force and displacement is nearly identical to the Hertz contact theory. In the current work, the KV model is compared initially with the theoretical results for a single viscoelastic bond. Then, elastic and viscoelastic spherical particle models including multiple bonds are developed and simulated under diametrical loading. Finally, applications of DMP to spherical particles composed of core and shell regions with different properties are also presented to demonstrate the potential for inhomogeneous systems. 2. Materials and Methods 2.1. Theoretical Background 2.1.1. Hertz Theory for Elastic Normal Contact Force Hertz proposed a theory to analyse the contact of two elastic isotropic spherical solids by assuming linear elasticity and frictionless boundary conditions [19]. For diametric compression, a spherical body is in contact with two flat surfaces, and the radius of curvature of the flat surfaces is set to infinity. Since the total deformation is evaluated, it is divided by two [20], and therefore, the relationship between the force, FH, and the relative displacement of the plates, δ, is as follows: √ FH = 3(E1 2υR2)δ3/2, − (1) where E, R, and υ are the Young’s modulus, radius, and Poisson’s ratio of the particle, respectively. 2.1.2. Viscoelastic Normal Contact Force For the diametric compression of a spherical viscoelastic particle, the force may be partitioned between the elastic deformation and the viscoelastic dissipation, thus [21,22]: FVE = Felastic + Fdissipative = Aδ3/2 + Bδ1/2δ, . (2) where δ and δ are the displacement and the rate of displacement, respectively. The elastic term is . the Hertzian contact force where A is the constant in the Hertz theory. The dissipative part has a dChisemsiEpnagtiinveeerincogn20s2t0a,n4t, xBFtOhRatPEwEaRsRdEeVrIiEvWed independently in [21,22,24]. 3 of 14 2.1.3. Mass-Spring-Dashpot Models 2.1.3. Mass-Spring-Dashpot Models Figure depicts two particles of mass connected by KV model, which is defined as ““KV„” bondFaignudriem1pdleempiecntstetdwnoupmaɑrtriiccdaelsIyoafsmdaessscrmibceodninnetchteednebxyt aseKctViomn.oWdehle,nwahiKchV ibaedndsdfiinseddisapslaaseKdVby baodnisdtaanncde iXmfprolemmeitnsteeqduniluibmrieurmicaplloysiatsIdne.stchrebreedsuilntinthgefonrecxet issegctivioenn. bWyhthene faolKloVwbinogndreilsatdioisnpslhaicpe:d by a distance x from its equilibrium position, the resulting force is given by the following relationship: FFK?V? == kkXX ++ bb ?d???t dX , (3) , (3) where is the spring constant and is the dashpot constant. If such force is applied to the model, the wdihsperleackeimsethnet swpirlilnbgecofnusntacntitoannodfbtiimseth,et,daasshopllootwcos:nstant. If such a force is applied to the model, the displacement will be a function of time, t, as follows: XX((tt)) = ?F?(11 ?− e−?k?b·?t??)?,, ?k (4(4)) Figure 1. Two particles connected by a spring and a dashpot in parallel. Figure 1. Two particles connected by spring and dashpot in parallel. 2.2. Model and Simulation 2.2. Model and Simulation In this section, we initially compare the numerical implementation of the spring and dashpot modeInlwthitihs tsheecttihoneo,rweteicianlirtieaslulyltscofomrpaasriengthlee vniuscmoeelraicsatilcibmopnIde.mTehnetnat,iwone eoxfttehnedstphreinsgtuadnydtodaaslhaprgoet gmeoodmeeltwryit(hspthheertihceaol)reinticclauldriensgulmtsuflotirpalesibnognledsv.iscoelastic bond. Then, we extend the study to a large geometry (spherical) including multiple bonds. 2.2.1. Validation of a Single KV Bond 2.2.1. Validation of a Single KV Bond The KV bond was implemented numerically in LAMMPS [25] following the standard Hooke’s law and NThewetKoVn’sbolanwd owfaflsuiimdpflloewmefonrtetdhensupmrienrgicaanlldydinasLhApoMt,MrePsSpe[c2t5i]vefolyll,oawsisnhgowthneisntaEnqduaartdioHno(3o)k.eT’os vlaawlidaantdetNheewnutomne’rsiclaawlimofpflelumidenftlaotwionfoorf the smparisns-gsparnidngd-dasahshppoot,trmesopdeeclt,iavesliym,palse sshyostwemn iwnaEsqcureaatitoedn (a3s).shToowvnaliindFatigeuthree1n,uamnderthicealdiimspplalecmemeenntattwioans ocfaltchuelamteadssfr-sopmritnhge-dsiamshuplaottiomnosdaenld, acosmimppalreedsytosttehme wanaaslyctriecaaltesdolaustioshnoowfEnqiunaFtiiognu(r4e).1T,hanedfotllhoewdinisgpplaacreammeentetrwvaalsuceaslwcuelraeteedmpfrloomyedthfeorsitmheusliamtiounlastiaonnds: Fco=m1pNar,emd t=o 0th.0e0a0n01alkygti,ckal=so0.I2utNio/nmo,fanEdquaartaionnge(4o).f Tvhaleufeoslloofwbi,nags sphaorawmneitnerFvigaulurees2w,werheereemmpliosytehde fmorastsheofsitmheublaetaiodns.s:TFh=e 1siNm,umla=te0d.0d0i0s0p1lakcge,mke=n0ts.2aNre/min,calnodseaargarnegeemoefnvtawluitehs tohfeb,aansalsyhtoicwalnsionluFtiigounr.e 2, whAerseecmonisd tvhaelidmaatisosnowftahsepberefaodrms.eTdhbeysicmomulpaateridngditshpelacrceeempeanntds arerceoivnercylorseespaognreseesmoefntthwesityhsttehme ainnaFliygtuicrael1sotloutthioant.calculated using Simulink (Version 9.1, The MathWorks Inc., Natick, MA, USA). 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Natick, MA, USA), as shown in Figure 4. Furthermore, in this case, the simulated ChemEngineering 2022002,04,,4x, 3F0OR PEER REVIEW 4 o4f 1o5f 14 ChemEngineering 2020, 4, x FOR PEER REVIEW 4 of 14 FFiigFguiugrrueer2e2..2C.oCmopmapraisroisnonoofoftfhtehedisplacement ccaalclcuulalateteddffrroommththeessimimuulalattioionnaanandnddthththeheaenanalayltyictiaclaslosIsouoltulioutnitoi,onn,, i.ie.e.i,..e,E.E,qquuaatitoionn((44()4)..). Figur3e. 3. Responsoef othfethe system depicteidn in Figur1e t1o tao a constant force, whichis is removed afte6r s. TFhi6geusb.rleuTeh3.eliRnbeelusipesoltnihnseeedoifsthpthelaedcseiysmpstleeanmctemcdaeelcpnuitclcataetledcduinlfartFoeimdguftrrhoeem1sittmoheuaslcaiomtinousnltaa,tnaiontndfo,trahcneed,rwtehdheilcrienhdeisliisrnecemailscoucvalealdctueadlfattuee STimhuesuibnlilgnukSe.imlinueliinskt.he displacement calculated from the simulation, and the red line is calculated using Simulink. A third validation was performed by comparing the displacement response of the system in Figure 1 to a sinusoidal load (dynamic force), to the value calculated using Simulink (Version 9.1, The MathWorks Inc. Natick, MA, USA), as shown in Figure 4. Furthermore, in this case, the simulated displacements were in close agreement with the calculated values. 2.2.2. Modelling the Diametric Compression of a Spherical Particle In DMP models, macroscopic bodies are sub-divided into computational particles (beads). Since in this work, we study KV bonds that can be used in DMP (or other particle-based multiphysics methods), we extended the validation to macroscopic spheres that accounted for multiple KV bonds. A sphere could be sub-divided into computational beads in different ways. Here, we employed two approaches: the beads were arranged on (a) a regular cubic lattice and (b) an irregular tetrahedral lattice. Figure 4. Response of the system depicted in Figure 1 to a sinusoidal loading force. The lines are the Figure 4. Response of the system depicted in Figure 1 to a sinusoidal loading force. The lines are the displacements calculated from the simulation, and the points are calculated using Simulink. displacements calculated from the simulation, and the points are calculated using Simulink. Figure 3. Response of the system depicted in Figure 1 to a constant force, which is removed after 6 s. ChemETnhgeinbeelruinegl2in02e0i,s4t,h30e displacement calculated from the simulation, and the red line is calculated using5 of 15 Simulink. ChemEngineering 2020, 4, x FOR PEER REVIEW 5 of 14 2.2.2. Modelling the Diametric Compression of a Spherical Particle In DMP models, macroscopic bodies are sub-divided into computational particles (beads). Since in this work, we study KV bonds that can be used in DMP (or other particle-based multiphysics metFhiogdusr)e,4w.eReesxptoennsdeeodf tthheesvyasltiedmatdioepnictotemdiancFroigsucroep1ictospahsienruessotihdaatl laocacdoiungntfeodrcfeo.rTmheullitniepslearKeVthebonds. A spdhiseprleacceomuelndtsbceaslcuubla-dteidvifdroemd tihnetosicmoumlaptiuotna,taionndatlhbeepaodinstsinardeicfafelcruelnattewdauyssin.gHSeirmeu,lwinek.employed two approaches: the beads were arranged on (a) a regular cubic lattice and (b) an irregular lattiIcne.the first case, the spherical particle (Figure 5a) was constructed from cubic lattice cells (Figure 5b). It contIanintheedf1ir3s7t,c0a5s9eb,tehaedsspwhietrhiceaalcphacrotinclnee(cFtiegdutroe 5thae)wneaasrceosntnsteriugchtebdoufrrosmancdubailconlagttfiacceecdelilasg(oFnigaulsre b5ybl)i.neItarcospnrtainingesdor13b7y,0K59V bbeoanddss.wTithhisewacohrkcofoncnuescetesdontovitshceoenlaesatriecsittyn(eKigVhbboounrdss)a,nadndaltohnegcafsaece odfipaugroenlyaleslbaystliicnsepahrseprersin(glisnoerarbsypKriVngbso)nwdas.sTchoimswpuotrekdfofocursceosmopnavriisscoone.laTshtiecictays(eKoVf lbionneadrs)s,parnidngths,e incafsaecto,hfapsubreeelyn eallarestaidcyspsthuedreiesd(,lainnedarmsapsrsi-nsgpsr)inwgacsubcoicmlaptutitceedcfeollrmcoomdeplasrairseonk.nTohwenctaosreeopfrelsineneatr (psuprreinlyg)se,lianstfiaccht,omhaosgbeeneonusailsroetardoypisctumdaiteedri,aalnsdif tmheascso-nspnreicntgiocnubbeitcwleaettnictehecemllamssoedsealnsdatrheeksntioffwnenstso orfetphreessepnrtin(pgsuraerley)seellaecsttiecdhaopmporogpenrioautesliyso[2tr6o]p.icFomraatecruiablisciflatthteicceocnenllecwtiiothn bneetawreesetnntehieghmbaosusres and ntehxet nsetiaffrnesets-sneoifghthbeousrprliinnegasrasrperisnegles,cttehde Paopipsrsoopnr’siartaetlyio[i2s6p].reFdoircteadcbuybitchelatthtiecoerycetlol bweit0h.2n5e[a2r6e]s,t annedigYhobuonugr’samndodnuelxutsniseagrievsetn-nbeyigthhbeofuorllloiwneianrgsrperlaintigosn,sthhiepP[2o7is]:son’s ratio is predicted by the theory to be 0.25 [26], and Young’s modulus is given by the following relationship [27]: E = 2.5 k/l (5) E = 2.5 k/l (5) wwhehreerel ilsisthtehelelnegntghthofoafnanedegdegeofotfhtehececlel.lll.nInththee“R“ReseusultlstsanadndDDisicsucsussisoino”n”(Sseeccttiioonn3,)o,uorumrmodoedlewlwillilble bieniintiiatilalyllyvavlaidliadtaetdedagaagianisntstthtehseestehtehoeroerteictaiclavlavlauleusefsofroar paeprfeercfetlcytleylaeslatisctiscpshpehreerbeyboynolynlayccaoccuonutinntginfgor folirnleinaerasrpsrpinrginsgasnadn,dl,altaetre,ri,titwwilillllbbeeextended ttooa viscoelastic sphere by substitutingththeesspprirninggsswwitihth KKVVbobnondds.s. (a) (b) Figure 5.5.(a(a))Visualisation ooffaaspherical particle between two parallel compression planes, which araere represented bybyrerdedlines; (b()ba)nanelementary ceclellolfoaf acubic lattice. The tetrahedral cells were created by discretising the sphere with a finite-element mesh generator. In this case, the distance between the beads was not perfectly uniform, and for this reason, we called it a disordered model. Using this approach, less beads were required, but the calculation of the elastic modulus a priori (Equation (5)) was less accurate [26]. A spherical particle based on a disorder model with 5921 beads was created using an open-source 3D finite element grid generator [28]. As in the case of the cubic lattice, the beads were connected to their neighbours either with linear springs or KV bonds to model, respectively, elastic and viscoelastic materials. The tetrahedral cells were created by discretising the sphere with a finite-element mesh generator. In this case, the distance between the beads was not perfectly uniform, and for this reason, we called it a disordered model. Using this approach, less beads were required, but the calculation of the elastic modulus a priori (Equation (5)) was less accurate [26]. A spherical particle based on a disorder model with 5921 beads was created using an open-source 3D finite element grid generator [28]. As in the case of the cubic lattice, the beads were connected to their neighbours either with linear springs or KV bonds to model, respectively, elastic and viscoelastic materials. Two parallel solid planes were applied to the particle in order to simulate diametric compression. They exerted a force to compress the particle, where the magnitude of the force, F(r), is given by [29]: F(r) = S(rb Ri)2, − (6) where S is the specified force constant, Ri is the position of the plane and rb Ri is the distance from − the bead to the plane. The force is repulsive, and F(r) = 0 for rb > Ri. The force constant was set to be 1010 Nm−2 for all simulations in order to represent rigid compression planes. During the compression loading simulations, one plane compressed the particle with a constant velocity for both the elastic and viscoelastic particle models, while the other was maintained static. For the viscoelastic particle, the displaced plane was held at its final position after the loading to allow for relaxation. The force and particle displacement were recorded during the simulations, and a time step of 10−11 s was used to integrate Newton’s equations of motion. It is well known that the KV model can produce the creep and recovery responses of a two-bead system, as shown in Figure 3, but cannot model stress relaxation behaviour. However, as will be shown in the next section, for the many-bead spherical particle models connected with KV bonds, stress relaxation behaviour could be observed. This is because a many-bead particle model connected with KV bonds is similar to a generalized KV model, i.e., a viscoelastic material model composed of N Kelvin–Voigt units assembled in series. The generalized KV model has been employed, for example to study the viscoelastic properties of micro-cracked materials [30]. 3. Result and Discussion 3.1. Perfectly Elastic Spherical Particles 3.1.1. Cubic Lattice Cell Model Figure 6a presents the simulated force as a function of displacement for an elastic spherical particle based on the cubic lattice cell with a spring constant of 200 Nm−1. The data were compared against the Hertz theory predictions (Equation (1)) and the comparison depicted in Figure 6b. The force and displacement calculated from the simulations were nearly identical to the Hertz theory. The fluctuating behaviour in Figure 6 was due to slight numerical inaccuracies that artificially perturbed the total energy of the system. Since the particle was perfectly elastic, this energy was never dissipated and manifested itself as a high frequency perturbation. This is a known issue with the LSM, which, in the literature, is usually solved by adding a small artificial dissipative term that damps these high frequencies [31]. In this study, since the focus was on validation, we did not implement any artificial dissipation. The calculated Young’s modulus for the spherical particle was 39.1 MPa, which was in a close agreement with the Young's modulus of the elementary cubic lattice cell of 40 MPa calculated using Equation (5). The small discrepancy arose because, due to the cubic cell internal structure, the bead model was not a perfect spherical shape, so that it did not fully comply with the Hertzian contact model. The bulk shear stress, which is the sub-surface principal stress difference, i.e., |(σ1 σ3)|/2, may be − calculated for each bead. The principal stresses (σ1 and σ3) were calculated from the virial stress and kinetic energy contributions [32] for each bead. The contours of the calculated shear stress are presented in Figure 7, where a is the contact radius and r is the particle radius. The shape of the particle based on the cubic lattice cell with a spring constant of 200 Nm−1. The data were compared against the Hertz theory predictions (Equation (1)) and the comparison depicted in Figure 6b. The force and displacement calculated from the simulations were nearly identical to the Hertz theory. The fluctuating behaviour in Figure 6 was due to slight numerical inaccuracies that artificially perturbed the total energy of the system. Since the particle was perfectly elastic, this energy was never dissipated and manifested itself as a high frequency perturbation. This is a known issue with the LSM, which, in the literature, is usually solved by adding a small artificial dissipative term that dcoanmtopusrtshwesaes shiimghilafrrteoqutheantcciaeslcu[3la1t]e.dInthtehoirsetsitcuadllyy, [3si3n,3c4e].thTehefomcauxsimwuamsovnalvuaelwidaastifoonu,nwdeatdaiddenpotht iomfp0.l5eam.eTnhtiasnisyianratifcilcoisael dagisrseiepmateionnt.with theoretical value of 0.48a [33]. ChemEngineering 2020, 4, x FOR PEER REVIEW 7 of 14 The bulk shear stress, which is the sub-surface principal stress difference, i.e., |(σ1 − σ3)|/2, may be calculated for each bead. The principal stresses (σ1 and σ3) were calculated from the virial stress and kinetic energy contrib(au)tions [32] for each bead. The contours of th(eb)calculated shear stress are preseFnigteudrei6n6..(Fa(i)agC)uorneta7c,t fworhcfeeorarecseafauissnctathioefnucnoocftndiotisanpcltaocfreamddieisunpstl;a(acben)mdcoernnttia;sct(tbfho)erccepoanasrtataiccftulenfocrtraicodeniuoafssd.aiTsphflueancsechmtioaenpnet3o/o2f.f the contodBuiosrtpshlawwceeamrseecsnaitml3c/2ui.llBaatroetdthofwrtohemraetthceaslcimulualtaetidofrnotshmoefoarnetesiiclmaaslutliylcast[ip3oh3ne,s3ri4oc]fa.laTpnaherelaticsmlteiacbxsaipsmehdeuromicnatvlhapelaucruteibciwlcealbasattsifecoeduconendll at a depthtmheoofdcue0lb..5iTca.hlaTetthdiciaseshicseedlilnlmianoecdsleoalsr.eeTthahegedrbeaeessmhtefiedtnsltionwfetsihtaherdethateaotrboeetsitcfaiHtlsveoraftlzuthteheoedofar0tya..4t8oath[3e3H].ertz theory. The calculated Young's modulus for the spherical particle was 39.1 MPa, which was in a close agreement with the Young's modulus of the elementary cubic lattice cell of 40 MPa calculated using Equation (5). The small discrepancy arose because, due to the cubic cell internal structure, the bead model was not a perfect spherical shape, so that it did not fully comply with the Hertzian contact model. Figure 77.. Contours of the sub-surface shear stresses estimated from the simulations using the cubic lattice cell. 3.1.2. Disorder Model 3.1.2. Disorder Model simuFlaitgiuonres 8uasipnrgetsheentdsisthoredneorrmmoadleclowntiathctafosprcreinags confustnacntitoonf 2o0f0dNispmla−c1e.mAeltnhtocuaglhcutlhaitsedinfvroolmvedthae Figure 8a presents the normal contact force as a function of displacement calculated from the ssmimaullleartinounmsubesirnogf tbheeaddsis,othrdeedramtaowdeerlewaicthloasesrpfirtintog acoHnesrtatznitanofre2s0p0oNnsme−(1FiAgultrheo8ubg)h,btuhtsiwiintvhoglrveeadter sflmucatluleartinounmsobfetrhoeffboeracde.s,Athsemdeanttaiowneerdeabcolovsee,rthfietsteofluHcteuratztiioannsrensopromnaslely(Fwigouurled8bbe),rbemutowveitdhwgritehataenr falruticfituciaatliodnissssiopfatthioenfoterrcme.,Abustminenthtiiosnveadlidaabtoiovne,etxhaemseplfelu,cittuisantiootneswnoorrthmyatlhlytaw,aosuelxdpbecetreedm,doivseodrdwerietdh astnruacrttuifriecsiainlcdreisassiepdattihoenatmerpmli,tubduetoifnththehipservtaulridbaattiioonn. eUxsaimngpEleq,uiattiiosnn(o1t)eawnodrathssyumthiantg, athsaetxup=ec0te.2d5,, disordered, structures increased the amplitude of the perturbation. Using Equation (1) and assuming the Young s modulus w,as calculated to be 12.4 kPa. that υ = 0.25, the Young s modulus was calculated to be 12.4 kPa. Figure 8a presents the normal contact force as a function of displacement calculated from the simulations using the disorder model with a spring constant of 200 Nm−1. Although this involved a smaller number of beads, the data were a closer fit to a Hertzian response (Figure 8b), but with greater fluctuations of the force. As mentioned above, these fluctuations normally would be removed with an artificial dissipation term, but in this validation example, it is noteworthy that, as expected, disordered structures increased the amplitude of the perturbation. Using Equation (1) and assuming that υ = 0.25, the Young's modulus was calculated to be 12.4 kPa. (a) (b) Figure 88..(a()aC)ontact forcefoarscaefuanscatiofnuofcdtiiosnpnlaocfemdeisnpt;la(bce)mceonnt;ct(fbo)rcceoanstaacfutnfcotriocen oafsdiaspfluacnecmtieonnt3o/2f. Bdoistphlwaceermeecanltc3u/2.laBtoedthfrwomeretthcealsciumlautleadtiofnrosmoftahne esliamstuiclastpiohnesricoaflapnaretilacsletichaspsphderoincatlhpeadritsioclredebramseodoeenl. Tthheeddiassohredderlimneosdaerle.Tthheefidtasoohfetdhleinsiemsaurleattehdedfiatstaotfo thesHimeurtlzattehdeodrayt.a to the Hertz theory. ChemEngineering 2020, 4, x FOR PEER REVIEW 8 of 14 Figure 9 presents the contours of the calculated sub-surface shear stresses, for which due to the randoFmigulorcea9tiopnreosfenthtes tbheeadcos,ntthoeuprsatotfertnhewcaaslcnuolattseimdisluarb-isnufroframcetsohtehaart sotfrethsseecsu,fboicr lwathtiicceh cdeullemtoodtheel. Hraonwdoevmerl,otchaetimonaoxifmthuembevaadlus,ethweapsaatltseornfowuansdnaott asidmeiplathrionffaobrmoutto0t.h5aatboeflothwe tchuebiscuIraftatcicee, wcehllicmhowdaesl. sHimowilaervteor, thecmubaixcimlauttmicevmaloudeewl.as also found at a depth of about 0.5a below the surface, which was similar to the cubic lattice model. FFiiegguurree 9.9.CoCnotnotuorusrosf mofaxmimaxuimmushmearshsteraerssbterensesatbhetnheeapthartlihclee spuarrftaicceleesstiumrfaatceed fersotmimtahteedsimfruolmatiotnhse osfimtheulaptaiortnicsloefbtahseedpaorntictlheebdaisseodrdoenr tmhoeddeils.order model. 3.2. Viscoelastic Spherical Particles 3.2. Viscoelastic Spherical Particles 3.2.1. Cubic Lattice Cell Model 3.2.1. Cubic Lattice Cell Model Figure 10 presents the contact force as a function of time during compression and relaxation calculFaitgeudrefro1m0pthreesseinmtsultahteiocnosnotfacatvfiosrccoeelastaicfsupnhcetrioicnalomfotidmeel bdausreidngoncothmepcruebsisciolanttaicnedcreelllladxuartiingn ccoamlcuplraetsesdiofnrowmitthheassipmruinlagticoonnssotafnatvoifsc2o0e0laNstmic−s1pahnedricaadlmasohdpeoltbcaosnesdtanttohfe1c0u−b6icNlmatt−i1ces.ceThldeuforirinceg acnodmdpirsepslsaicoenmweintthda... rwinegrecfiotntsetdantot oEfq2u0a0tiNonm(2−1)ainndoraddearsthopoobttacionntshtaenvtaolufe10o−f6 AN,man−1ds.hTehnecefoYro...agn'ds mdiospdlualcuesmuesnintgdaEtqauwateiioenf(it1t)e.dIttowEasqufoautinodn t(o2)bie...d8eMrtPo...bthaiinchthweavsaslluigehotlfyAl,esasndthhanentcheatYfoourntgh'es emiosdtiuclpuasrutis:ilneg. Equation (1). It was found to be 36.8 MPa, which was slightly less than that for the elastic particle. An analysis of the force relaxation after compression was performed using a previous method for experimental compression of an agarose micro-particle [35]. Instantaneous (E_0, corresponding to t = 0) and long-time (E_∞, corresponding to t = ∞) elastic moduli were then calculated. The values were found to be E_0 = 54 MPa and E_∞ = 34 MPa. The Hertzian Young's modulus was close to the calculated relaxed value. The relaxation times are t_1= 0.49 s and t_2= 4.6 × 10−5 s. modulus using Equation (1). It was found to be 36.8 MPa, which was slightly less than that for the elastic particle. An analysis of the force relaxation after compression was performed using a previous method for experimental compression of an agarose micro-particle [35]. Instantaneous (E_0, corresponding to Cth=em0E)nagnindeelroinngg2-0t2i0m,4e, 3(E_0, corresponding to t = ∞) elastic moduli were then calculated. The values9wofe1r5e found to be E_0 = 54 MPa and E_∞ = 34 MPa. The Hertzian Young's modulus was close to the calculated relaxed value. The relaxation times are t_1= 0.49 s and t_2= 4.6 × 10−5 s. Figure 1100.. Contact force aass a function ooff time during compression and relaxation calculated from tthhee simulations oofftththeeviscoelastic spherical particle bbaasseeddoonntthheecuubbicicllaltttitciceecceellllmmooddeel.l. An analysis of the force relaxation after compression was performed using a previous method for experimental compression of an agarose micro-particle [35]. Instantaneous (E0, corresponding to t = 0) and long-time (E∞, corresponding to t = ∞) elastic moduli were then calculated. The values were found to be E0 = 54 MPa and E∞ = 34 MPa. The Hertzian Young's modulus was close to the calculated relaxed value. The relaxation times are t1= 0.49 s and t2= 4.6 10−5 s. × ChemEngineering 2020, 4, x FOR PEER REVIEW 9 of 14 3.2. 2. Disorder Model 3.2. 2. Disorder Model Figure 11 presents the simulated contact force as a function of time for a viscoelastic spherical 1p0a−r6tiNclme−b1asse.dThoenftohrceedainsodrddeisrpmlaocedmelewntitdhaataswpreirnegfictotendsttaonEtqoufa2t0io0nN(2m)−i1naonrddeardtoasohbptoatincothnestvaanltuoef particFleigbuarseed11opnrtehseentdissothrdeesrimmuoldaeteldwcitohntaascptrfionrgcecoasnsatafunntcotfio2n00oNftmim−e1 afonrda vdiascsoheploasttciocnsspthaenrticoafl o1f0A−6, Nfrmom−1 ws.hTichhe tfhoercYeoaunndg,dsimspoldacuelmusewntadsaotbatawineered fuitstiendg tEoqEuqautiaotnio(n1)(a2s) 1in12oKrdPear, twohoibchtawinatshgerveaatleure tohfanAt,hferocmalcwulhaitcehd tvhaeluYeofuorngth'se melaosdtiuclupsarwticalse.obtained using Equation (1) as 112 KPa, which was greater than the calculated value for the elastic particle. Figure 11. Contact force as a function of time during compression and relaxation calculated from the sFimiguulraeti1o1n.sCoofnthtaecvtfisorcoceelaasstaicf...hcetiroicnaolfptairmtiecldeub...egdcoonmtphreedssiisoonrdaenrdmroeldaexla.tion calculated from the simulations of the viscoelastic spherical particle based on the disorder model. An analysis of the force relaxation after compression was performed using the procedure used for the cuAbinc alantatilcyesimsoodfethl.eTfhoerceelarsetliacxmatoiodnulauftsevra...nuwndastopebrefoE_0m=ed20u3sKinPgatahnedpEro∞ce=d2u0r0e KusPead. Tfhoer tHheerctuzibainc lYaottuicnegm'somdoedl.uTlhues ewlaasstilcesmsothdaunlutshveaclaulecsulwateerde froeulanxdedto...n=d2i0c3atKinPga tahnadt t...f=or2c0e0 KPa. The Hertzian Young's modulus was less than the calculated relaxed value, indicating that the force was not fully relaxed after compression. The relaxation time t_1 = 0.82 s and t_2= 2.83 × 10−5 s. It is noteworthy that since the dashpot accounted for the physical viscosity of the material, artificial dissipation was not necessary in these examples. 3.3. Application of the Elastic Disorder Model: Hard Core-Soft Shell and Soft Core-Hard Shell Spherical was not fully relaxed after compression. The relaxation time t1 = 0.82 s and t2= 2.83 10−5 s. It × is noteworthy that since the dashpot accounted for the physical viscosity of the material, artificial dissipation was not necessary in these examples. 3.3. Application of the Elastic Disorder Model: Hard Core-Soft Shell and Soft Core-Hard Shell Spherical Particles under Compression In this section, we consider spherical inhomogeneous particles composed of a hard core-softer shell (HC-SS) and a soft core-harder shell (SC-HS). The models were based on a disorder lattice with 6065 beads. The beads were connected with springs to their neighbours. The hard regions of the particles were modelled using a larger spring constant than that for the soft part. The ratios of shell thickness, h, and the particle radius, r, were set to be 0.5, 0.2, and 0.05. A visualization of the shell thickness and particle radius is presented in Figure 12. A small artificial damping force (1−10 Nm−1.s) was added to the beads, which was proportional to the relative velocity of the beads, in order to damp the kinetic energy from the system and obtain a smoother compression force. Two parallel solid planes were positioned on the surface of the particle in order to simulate diametric compression, as described in the previous section. Using Equation (1) and assuming that υ = 0.25, the Young's modulus was CcahelmcuElnagtiendeerfiongr 2e0a2c0h,4c,xasFeO.R PEER REVIEW 10 of 14 Figure 12. Illustration of shell thickness (h) and particle radius (r). Figure 13 presents the force as a function of fractional deformation (δ/2r) of HC-SS particles with different values of kcore and h/r. Figure 14 presents the force as a function of fractional deformation (δ/2r) of SC-HS particles with different values of kshell and h/r. The force profiles in Figures 13 and 14 can be compared with experimental data to simplify theoretical equations for small deformation e.g. for microcapsules [36]. By comparing Figures 13a and 14a, for the deformation up to 5%, it may be seen that the change in kshell affected the deformation force more significantly than the change in kcore. Figure 13a shows that by reducing kshell from 200 to 20 Nm−1, the deformation force is now just about 11% of the initial value; while in Figure 14a, by reducing lcore from 200 to 0.2 Nm−1, the force now is about 67% of the initial value. Thus, at small deformations, the compression load is mainly absorbed by the shell. Increasing the h/r ratio from 0. 05 to 0.2 changed the deformation force more significantly than increasing the h/r ratio from 0. 2 to 1, as presented in Figures 13b and 14b for the deformation up to 5%. Increasing the h/r ratio from 0. 5 to 1 did not change the force significantly. Moreover, it may be seen from Figures 15b and 16b that changing the h/r ratio from 0.5 to 1 did not change the lumped Young's modulus significantly. In(tah)ese cases, the h/r ratio of 0.5 could be consid(ebr)ed as a cut-off ratio where thereFwigouureld13b.e(an)oThsiegfnoirficecaanstacfhuanncttgioentoftfhreacmtioondaulldueesf.ormation (δ/2r) of HC-SS particles (h/r = 0.2 and different kshell) and a hard solid particle (kshell = kcore = 200 Nm−1). (b) The force as a function of fractional deformation (δ/2r) of HC-SS particles (kcore = 200 Nm−1 and kshell = 20 Nm−1) with different values of h/r and a soft solid particle (h/r = 1, kcore = kshell = 20 Nm−1). Figure 12. Illustration of shell thickness (h) and particle radius (r). (a) (b) FigurFeig1u3r.e (1a3). (Tah)eThfeorfocerceasasaa function oofffrfarcatciotinoanladlefdoermfoartmioant(iδo/n2r)(δoo/ff2Hr)Co-SfSSlepsa(rht/irc=le0s.2(han/rd= 0.2 and ddiiffffeerreenntt kkshsehllle)lla)nadnadhaarhdasrodlisdopliadrtipcalert((ikkcsshhleeelllll =(kkkscchoorreeel=l =20k0coNrem=−−11))2..0(b0)NThme−f1o)r.ce(ba)s Tahfuenfcotircne ooaffsfarafcutinonctailon of fvraalcuteidaosnenofdaoflrahmds/reoafftaotinosrnodml(iaδad/ts2ipoora)fnrtoot(isffcδoHl /el2iCr(dh-)S/porSaf=prH11tai,,rCckktlic-cecooSrrlee(eS=hs /pkkr((sskkahh=cceeroolllllrrtee=i1=c,2l2ke00csNo0r(emNkc=mo−−11r)ek)−−..s11=haenl2ld0=0kk2ssNhh0eellllm=N−2m10−Na1nm)d.−−11k)swhelilth=d2if0feNremnt−v1a)lwueisthooffdhi/ffrerent ChemEngineering 2020, 4, x FOR PEER REVIEW 11 of 14 By comparing Figures 13a and 14a, for the deformation up to 5%, it may be seen that the change in kshell affected the deformation force more significantly than the change in kcore. Figure 13a shows that by reducing kshell from 200 to 20 Nm−1, the deformation force is now just about 11% of the initial value; while in Figure 14a, by reducing lcore from 200 to 0.2 Nm−1, the force now is about 67% of the initial value. Thus, at small deformations, the compression load is mainly absorbed by the shell. Increasing the h/r ratio from 0. 05 to 0.2 changed the deformation force more significantly than increasing the h/r ratio from 0. 2 to 1, as presented in Figures 13b and 14b for the deformation up to 5%. Increasing the h/r ratio from 0. 5 to 1 did not change the force significantly. Moreover, it may be seen from Figures 15b and 16b that changing the h/r ratio from 0.5 to 1 did not change the lumped Young's modulus significantly. In these cases, the h/r ratio of 0.5 could be considered as a cut-off ratio where there would be no significant change to the modulus. Based on the results, a(lau)mped Young's modulus could be calculat(ebd) using Equation (1), which rFeipgurerFseiegn1u4tre.ed(1at4h).e(Tae)hqTeuhfieovrafcoleercnaetsaYsaoaufunngc'stimonoodofuflfurasctthioenpaalrtdicelfeorwmoautl(idδo/n2hra)(vδoo/ef2fiSrfC)it-oHwfSSepCrea-rHhtiocSmlepsoa(grhte /rinc=leeo0s.u2(sha.n/Frdi=gu0r.e2 1a5ndanddiffFeigreunrtekkc1ocr6eo)repa)nredasnaednhatartdhhesaorlldiudmspopalierdtdicplYeao((rkuktccoinorcreegl=e'sk(shkmecll)oo.red(bu=)lTikhoshefelfHlo)r.Cce(-SbaSs) aTanfhudencSftoCior-cnHeooSaffsfpraaacrtftiuiocnnleacsltidaoesnfoaorfmfufanrtcaiotcintoionnoafl khsaherldlo(srho/krlci=odre11,p,,takhkcrcoeotrreieYc=loekkusshh(eenhllll/g=r'2s=0m01,Nokdmcou−r−1l1eu))..=s kinshcerlle=as2e0s0foNrmH−C1-)S.S and SC-HS particles, respectively. For the HC- kdseheflolaroomnffdSaCtki-cooHrne,SorpefasSrptCiec-clHetisvS((ekkpclcooyraree,r=tai2ncNldemsa(s−−11kackkosshhrfeeeulll=nc22t0i0NonNmmo−f1t)khwsehietlhhl/=rdir2faf0etr0ioeNn.tAmvsa−le1ux)epsweooicfftthhe /drd,aiffwndeirtaehnhiatnrvcdraesloualseiidsnpogafvrhtai/crluleaensdoaf SS particle, increasing the h/r ratio decreased the Young's modulus, while for the SC-HS particle, it increased the value. (a) (b) FigurFeig1u5re. 1(5a.)(La)umped Young's modulusooff HC-SS particloefsFoigfuFreig1u2area1s2aafuansctaiofnuonfctkisohelnl. (obf) kshell. (b) Lumped Young's modulusofof HC-SS particloefsFoigfuFriegu12rbe a1s2ba fausnactfiounncotfiho/nr.of h/r. (a) (b) ChemEFnigginuereerin1g5.20(a20),L4u,3m0ped Young's modulus of HC-SS particles of Figure 12a as a function of kshell. (b1)2 of 15 Lumped Young's modulus of HC-SS particles of Figure 12b as a function of h/r. Figure 16. (a) Lumped(aY)oung's modulus of SC-HS particles of Figure(1b3)a as a function of kcore. F(big).uLruem16p.e(da)YoLuunmgp'sedmoYdouulnugs'sofmSoCd-HulSuspaorftiScCle-sHoSf Fpiagrutircele1s3bofaFsiagufurenc1t3ioanaosfah/fru.nction of kcore. (b). Lumped Young's modulus of SC-HS parti,cles of Figure 13b as a function of h/r. Based on the results, a lumped Young s modulus could be calculated using Equation (1), which represented the equivalent Young's modulus the particle would have if it were homogeneous. Figures 15 and 16 present the lumped Young's moduli of HC-SS and SC-HS particles as a function of kshell and kcore, respectively, and as a function of the h/r ratio. As expected, with increasing values of kshell or kcore, the Young's modulus increases for HC-SS and SC-HS particles, respectively. For the HC-SS particle, increasing the h/r ratio decreased the Young's modulus, while for the SC-HS particle, it increased the value. 4. Conclusions It has been demonstrated that the LSM could accurately represent the deformation, including the associated sub-surface stress fields, not only for elastic particles, but also for viscoelastic particles when linear springs were substituted with KV bonds. The disorder model was computationally more efficient than that based on a cubic lattice cell and led to a more refined definition of particle shape. Although only spherical particles were investigated in the current study, the approach is readily applicable to more complex shapes of the type that are often encountered in the pharmaceutical sector. The proposed technique could be employed, within a particle-based multiphysics model such as DMP, to model mechanical inhomogeneity, for example the softening of a particle immersed in water could be modelled by coupling the Young's modulus with the diffusion coefficient. It could also be extended to non-linear elastic deformation, plastic deformation, and fracture by introducing non-linear springs, friction elements, and springs of limited extensibility. For example, the fracture strength is of particular interest for encapsulates. If compared with gluing DEM particles together to model different shapes, the proposed technique provided not only accurate contact stresses, but also the stresses within the particle. The disadvantage, however, was in the greater computational cost. However, it was considerably more convenient to implement than discrete finite elements, which require more complex material models. The proposed approach could also be adopted to develop effective interaction laws for inhomogeneous systems in DEM simulations to reduce the computational cost. It would also be possible to incorporate LSM particles in a DEM simulation. Author Contributions: Conceptualization, I.H.S., A.A., and M.J.A.; methodology, I.H.S., A.A., and M.J.A.; software, I.H.S.; validation, I.H.S.; writing, original draft preparation, I.H.S; writing, review and editing, I.H.S., A.A. and M.J.A.; funding acquisition, A.A. and M.J.A. All authors read and agreed to the published version of the manuscript. Funding: This research was funded by Engineering and Physical Sciences Research Council, Grant Number EP/ M02959X /1. Acknowledgments: The computations described in this paper were performed using the University of Birmingham's BlueBEAR HPC service, which provides a High Performance Computing service to the University's research community. See http://www.birmingham.ac.uk/bear for more details. Conflicts of Interest: The authors declare no conflict of interest. Nomenclature a contact radius API Active Pharmaceutical Ingredients b dashpot constant δ relative displacement δ . rate of displacement DEM Discrete Element Method DMP Discrete Multiphysics E Young's modulus F force F(r) force (diametric compression) FE viscoelastic normal contact force FH force (Hertz theory) FKV force (Kelvin–Voigt model) h shell thickness HC-SS hard core-softer shell k spring constant KV Kelvin–Voigt l length of an edge of the cell LSM Lattice Spring Model m mass r radius rb-Ri distance from the bead to the compression plane Ri position of the compression plane σ1, σ3 principal stresses S specified force constant SC-HS soft core-harder shell υ Poisson's ratio X distance from equilibrium position References

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