RelationshipsbetweenBreakthroughCurvesandX-rayComputed TomographyAnalyzedMacroporeCharacteristics

TenundisturbedsoilmonolithsofclayeyPelosolatGottingen,GermanycoveringthehorizonsA_bandPwerecollected .Somecolumnswereleftatnaturalhumidity,somewereoven-driedtosimulatedrought situationsinforestsoilsinconsequenceofclimatechange.Insevencolumns,fourmicro-lysimeters,each, were installed at half height in order to obtain data for analysis of single solute pathways. A fixed amountofKBrtracerwasappliedtothehumuslayer.ThecolumnswereirrigatedwithCaCl₂.Columnoutputand lysimeteroutput we recollected and analyzed to record break through curves. Bimodal analytical convectiondispersionequation(CDE)solutionswerefittedforthecolumnoutputsusinganon-linearleastsquarefit. AsimpleCDE solution did not fit well. This supports the model of two overlaying transport phenomena.Afterbreakthroughrecordingwascomplete, all columns were scanned using X-ray computed to mography (CT).FromtheCTdata3-Dreconstructionsoftheporoussystemwerecreatedforvisualinspection, and the exact pathways form a cropores along them icro-lysimeters were determined. Additionally, indices of the pore structure we recomputed to compare with the slow and fast dispersivity values from the bimodal structure we have the structure of tCDEfit.Thevariationinmicro-lysimeterperformancecouldbeexplainedusingthe3-Dreconstruction. Statisticallysignificantdifferencesbetweentheporestructureofwetanddriedcolumnsaftertheendof irrigationcouldnotbeidentified. The pore index has generally an egative linear relationship with the fast dispersivity, and a positive linear relationship with the slow dispersivity. These relations are stronger in topsoil.TheCTpicturesand3-Dre-constructionsprovideaninterestinginsightintothesoilporesystem andmayhelptounderstandman-madedroughtproblemsduetoclimatechange.

Keywords: Tracertransport, X-ray computed tomography, 3-Dvisualization, bimodality, CDE, dispersivity, BTC/breakthrough curves

Themainresearchquestionofthisworkwastofind out,ifsinglepathwaysinunsaturatedflowofwetand driedsoils(withregardtodroughtsduetoclimate change)couldbecharacterizedintheirfunctions. Quantitativerelationshipsbetweensoilstructure (especiallymacroporecharacteristics,namelytheirsize, number,type,distributionandcontinuity)and soilhydraulicpropertiesareessentialforimproving ourabilitytomodelflowandtransportinstructured soils.Bouma(1979)andothershaveusedchloride breakthroughcurvesfromundisturbedsoilcolumns asanindirectmeansofcharacterizingmacropores.In recentyears, X-ray computer tomography (CT) data, which is based on varied linear attenuation of water, airandsolidmaterials, provided an attractive tool for soilscientiststonon-invasivelyobservesoilstructure (GantzerandAnderson2002;Luoetal.2008;Taina etal.2008;Kumaretal.2010).Warneretal.(1989) usedCTdatatoinvestigatethemacroporesystem, e.g.characterizationofcracks,earthwormholesand rootingchannels.Peytonetal.(1992)concentrated onmacropores, quantifying macropore perimeters, the pathsurroundingmacroporeshapes.Arelationship betweenmacroporesvisualizedbyCTdataand preferentialflowwasinvestigatedbyHeijsetal. (1996).Luoetal.(2010)relatedmacropore characteristicsquantitativelytosolutetransport parametersundersaturated conditions. Borges and Pires(2012)havestudiedtherepresentative

Columnnumber	Treatment (type)	watercontent(%) (mean)	Br-Pulset ₀ [day] (Bramount[mg])	Recoveryrate(%)
1-4	Naturalhumidity (1)	37.5	0.833 (14.9-16.4)	76.9-85.9
5-7	Oven-dried (2)	30.7	0.833 (15.8-18.3)	55.2-91.1
10-12	Oven-dried (3)	30.7	0.0833 (15.3-17.3)	46.6-68.0

Table1.Descriptionofexperimentaldesign

elementaryarea(REA) ofsoilsamplesusingCTdata, andconcludedthatsampleswithvolumesfrom50 cm³to100cm³withminimumcrosssectionof640 mm²areenoughtoberepresentativeforthesoil structure.Oursoilsampleshadvolumesofabout5000 cm³withacrosssectionof169cm².

ThepresentstudywascarriedoutatUniversity ofGöttingen,InstituteforSoilScienceandForest Nutrition,Büsgenweg,Germanyonsoilcolumnsofaclaye vPelosol(VerticCambisol)withwelldescribed swellshrinkcharacteristics(Spangenbergetal.2011).Theobject ivesweretostudytheroleofporecontactofmicrolysimetersinthesoilcolumnontracertransportinrelationt othestructure, as assessed by XrayCTunderdifferentinitialconditionsand irrigation.Asitisnotpossibletocarryoutthese investigationsunderfieldconditions, non-destructive CTdatawereused, makingitpossible for 3-Dreconstructionofthestructureoftheinvestigatedsoil columns.Furthermore,usingCTdata,anattemptwas madetounderstandtherelationshipbetweenthe breakthroughcurvesofthetracers(velocity, dispersionanddispersivity)andthemeasuredvolume and structure of the pores.

MaterialsandMethods

Thesoilstudied

ThesoilinthepresentstudyisaclayeyPelosol(Vertic Cambisol), developed from Muschelkalk (shell-lime) plate auderived from Triassicsed iment layers. Collected horizons were $O_{l(f)}$ - A_h - P, $O_{l(f)}$ was removed, only A_h -Premained. The Phorizon showed apolyedric structure (loamy clay). In this horizon, swell-shrink characteristic sare well expressed, and swelling clayminer alsaccounted for 26±5 %. Mineral compositions show quartz, illite, corrensite, or tho clase, albite and goethite. The details of the soils and the experimental setup we regiven in Spangenberg *et al.* (2011). A representative sample was taken in the area where the soil columns we regive the source of the source of the soil columns we regive the source of the soil columns we regive the source of the source of the soil columns we regive the source of the source

taken.Thissamplewasanalyzedforsoildensityin variousdepths.Bulkdensityrangedfrom0.908Mg m⁻³(topsoil,A_h)to1.569Mgm⁻³(subsoil,P,20-30 cmdepth).

Thecolumnexperiment

Originally, twelve undisturbed soil columns we rec ollectedinplexiglasscylindersof14.7cm diameterandabout30cmheightfroma4m2sampling area.Tencolumnswereselectedforthisstudy,butin ordertoreducethetotalamountoffiguresonly columns1,5and12arepresentedanddescribedin detail.Table1showsanoverviewoftheexperimental design.Fourcolumns(1-4)werekeptattheirnatural meanwatercontentofabout37.5%(meanvalue, n=4).Columns5-7and10-12weredriedat105°Cin aheatingcabinettoawatercontentof30.7%(Table1).Four micro-lysimeters.each.wereinstalledin sevensoilcolumns.Thesemicro-lysimeterswere equippedwithahydrophilicporouspolymertube (diameter2.3mm), madebyEijkelkampAgrisearchEquip ment, Netherlands (Spangenbergetal. 1997). Theyweredesignedspecificallytominimizethe impactofinstallationintosoil. Theywere installed at abouthalftheheightofthecolumninordertoallowobservati onoftheflowparametersinhighertemporal and spatial resolution in addition to the bottom output. Allcolumnswereirrigatedinavacuumpacked plexiglascontainer, which is a complete soil microcosm(describedinSpangenbergetal.2011). Irrigationwasappliedusinganelectronicdeviceevery 2h.Atthebottomofeachmonolith,unsaturatedflowwasadj ustedto300hPa.Abromidepulsewasapplied toeachcolumnatthebeginningoftheexperiment. ThenregularirrigationwithCaCl₂wasstarted, which lastedforatleast30days, i.e. untilnomore bromide wasfound in the column output. Solutions amples we recolle cteddailyatthebottomandfromthemicrolysimetersofeachcolumn.Theywereanalyzedfor chlorideandbromide.AnalysesweredonebyHPLC ionchromatography.Elutionmixturecontained

Na₂CO₃(2mmol)andNaHCO₃(0.75mmol). Detectionlimitofbothelementswas300µgL⁻¹.The statisticalanalysiswasdoneusingSAS(Statistical AnalysisSystem,SASInstitute,Inc.,Cary).The procedure"nlin"ofSASwasusedtoprovideleast squaresmodeling.Ananalyticalsolutionofthe convectiondispersionequation(CDE)wasusedtofit thebreakthroughcurvesoftheexperiment(vanGenucht en1982).Modelparameterswereestimatedusingbimodal ity,sinceitresultedinthebestfit (Spangenberg*etal*.2011).

BTCModeling

Themostimportantmodelforsolutiontransport insoildescribesconcentrationchangesintimeand spaceusingtheCDEaccordingtoNielsenandBiggar(1962).

$$R\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2} - v\frac{\partial C}{\partial x} \qquad \dots (1)$$

where,*C*=concentration[ML⁻³];*t*=time[days]; *x*=spatialdistance[L];*D*=dispersioncoefficient; *v*=averageporevelocity[LT⁻¹]

$R = \text{Retardation}(\text{dimensionless}) \qquad R = 1 + \frac{\rho_b K_d}{\theta} \qquad \dots (2)$

where,

 ρ_b =soildensity[ML⁻³]; K_d =constantfactor[L³M⁻¹]; ρ =volumetricwatercontent[L³L⁻³]

AccordingtoToride*etal*.(1995)Rcanbeset on1. Starting(1.0)andboundaryconditions(1.1and 1.2)are:

$$C(x,0) = C_i$$
 ...(1.0)

$$\left(-D\frac{\partial C}{\partial x}+\nu\right)|_{x=0} = \begin{cases} \nu C_0 \ 0 < t \le t_0 \\ 0 \ t > t_0 \end{cases} \qquad \dots (1.1)$$

$$\frac{\partial C}{\partial x}(\infty, t) = 0 \qquad \dots (1.2)$$

Assumingalteredinfiltrationanddisturbedwaterflo wduetosoildroughttheconditionsforapplication oftheCDEontreatmenttype2and3(Table1)were incomplete.Butconcentratingontheaimofthe investigation-acomparisonbetweendifferent experimentalvariantsofdriedandhumidsoils-the samemethodsofdataanalysishadtobechosen.To considerdifferentflowbehaviorofdriedandnondriedsoilsomenewboundaryconditionsfortheuse ofananalyticalsolutionoftheCDEwereinvolved (NielsenandBiggar1962).Abimodalvariantofthis CDEwasused,moredetailsonthispartareprovided inSpangenberg*etal.*(2011).

X-raycomputedtomography

Aftertheirrigationphase, the columns with installedmicro-lysimetersweretomographedina HospitalofGoettingenUniversity.AmedicalCTscanner (HiSpeedAdvantage,GeneralElectric)wasused.Forthep urposeofour30cmlongsoilcolumns, theheadnecksettingswerechosen.Tounderstand the differences between moist and dry treatments, each soilcolumnwastomographedindividually.Theoutput oftheCTunitisinHounsfieldUnits(HU), which is an intern ationallystandardizednumberingscale (Petrovicetal.1982). The numerical value of HounsfieldUnitdependsontheattenuation coefficients of the subject matter relative to that ofwater(Hainsworth1983;Greversetal.1989;Heijset al.1995), which is given as H=1000(μ - μ_w)/(μ_w - μ_a). Here, µisthelinearattenuation coefficient of the materialorpixelinguestion, u, and u, are the attenuationcoefficientsofwaterandair, respectively. A512by512matrixofpixeldatawasobtainedfor eachscan.Apixelhadthewidthofabout0.76mm. Thescanwastakenatintervalsof2mm(ca140 scanspercolumn).Aconstant1000wasaddedto everyvalue, which is used on all CTs canners, and giveninformulaforH.Afterthisaddition.airhasa valueof0andwater1000.Foreachpixel,theX-ray attenuationvalueswerestoredasvaluesfrom0to 4095.Thisrangewasduetothe12-bitprocessingof thetomographyequipment. The high values correspon dtothemetalofthemicro-lysimeter.The PV-WAVEwasusedforcomputeranalysis, which allowedreconstructing, visualizing and quantifying 3-Dmacroporestructureinthesoilcolumn(Pierretet al.2002).

Indicatorsforporestructure

ThemostimportantoutcomeoftheCTdataistheinfor mationonthecontentofsolidsandsoil porosity.The12bitdatawasreducedto8-bitdata andthewholedatasetwasscaledbydividingallthe valuesbyafactor16,sothatwehavevaluesranging from0-255.Goodspatialresolutioncanbeachieved whenthereisalargedifferenceinHvaluesbetween asubject(*e.g.* asoilpore)andthebackground(*e.g.* soilmatrix)assuggestedbyGrevers*etal.*(1989).

Inthepresentstudy, the same interior region of the top-

and subsoil in all the soil columns was selected, the area aro und the micro-

lysimeterswasintentionallyleftout. Theselected interiorr egionswered ivided intoroughly cubicareas. These cubes f orm the basis for further data processing. I deal cubes



butionofX-rayattenuationvaluesàseparationofsoil solidsandair;determinationofsoilsolids–(grayareas showtheextentofsoilsolids);cubesize2×2cubesize 4×4cubesize8×8countingofcubeswithhighairvolumes(whitecubeshavemorethan75%airvolume)

arenotpossiblewiththegivenvoxelsize.Therefore, differentsizeswereconsidered,namely,[4,4,1]voxel (labeled2×2),[8,8,2]voxel(labeled4×4)and[16,16, 4]voxel(labeled8×8).Thesecubescorrespondto volumesfrom18mm³toabout1cm³.Thestepwisecalculationforthe3cubesispresentedinfigure1.

 $\label{eq:second} First a threshold was selected to distinguish between densematter and pores. A value of 110 was selected, as this provided the best separation based on known material locations. The percentage of cubes with less than 25% denses oil was computed for each sample area and cubesize, which are labeled P_1, P_2 and P_4, de pending on cubesize. These we reused as indexes for the pore structure of a column. For a completely homogeneous material, all indexes would be the same. We used P_1 as an index for the fine pore structure and P_4 is an index for the coarse pore structure. The index esdon ot represent the connectivity of porous volume, only the amount of$

poresataspecificscale. The dispersivity values from bimodal tracer description were related to the seindices f or pore structure at three different scales. The seindices we recompared to the dispersivity results of the CDE models.

3-Dreconstructionofsoilstructure

Inthecoreofthecolumn.whichhasacrosssectionalareaofabout10cm×10cm.thevoxelswithscaled attenuationvaluesfrom0to30were reconstructedasa3-Dimageofsoilstructure. This allows avisual inspection of p oreconnectivityfor qualitativeanalysis.Avalueof30waschosento allowtheair-filledinnerpartsofmacroporestobe visible.Forabetterviewoftheporecontactofeach lysimeter, the slice with the lysimeters was reconstruct edseparatelyinthreeviewingangles(40°, 70and85°) with same viewing angle in all cases, *i.e.* forallcolumns(Figs.2,3and4).However,only slicewith40degreesviewanglewaspresented.In ordertoovercometheeffectofairpocketsinthe outerspacearoundthesoilcolumn, the central square areaof10cm×10cmwasselectedforthe3dimensional reconstruction. At the top as well as at thebottomsomeslicesofthecolumnwerediscarded. Thelocationofthemicro-lysimetersinthecolumn wereestablished, inwhichthex-, y-andzcoordinatesofthelysimeterheadandterminalinthe crosssectionimageweredetermined.

ResultsandDiscussion

Influenceofplacementofmicrolysimetersandtheirfunction

Thesuctionlysimetersofthetracerexperiment draindifferent quantities of solution, although during theentireconductoftheexperiment, as uction of 0.030MPawasmaintained. The great variability in thequantityofdrainedsolutionappearstobecaused bythedifferenceinpositioningofthemicrolysimetersinthecolumns, relative to the porous system of t hecolumn.Preferentialflowmayinitially havebypassedthelysimetersaltogether, butrelative positiontotheporoussystemseemstohaveahigh influence.Inordertoexplainthisphenomenon,one columnineachgroupispresentedinfigures5,6and 7.Eachfigurecontainsacrosssectionimageatthe heightofthemicro-lysimeters, aschematicofmicrolysimeterplacementandthedailyamountsofsolution drained.Thefiguresareusedtojudgetherelativesuctionpe rformanceofthelysimeters.Allfour lysimetersof column1showsimilarperformance(Fig.



Fig.2a,Column1,withsection



Fig.2b,Column1,section,40degree

 $\label{eq:Fig.2.3-D} Fig. 2.3-Dreconstruction of column 1 (experimental variant 1) within stalled micro-lysimeters. In the core of the column, the scale dattenuation values from 0 to 30 are presented. For abetter view, the section with the lysimeters is presented in a 40 degree look-angle. The core of the column has a cross-section alarea of 10 cm \times 10 cm$



Fig.3a,Column5,withsection



Fig.3b,Column5,section,40degree

Fig.3.3-Dreconstructionofcolumn5(experimentalvariant 2)withinstalledmicro-lysimeters.Inthecoreofthe columnthescaledattenuationvaluesfrom0to30are presented.Forabetterview,thesectionwiththelysimetersispresentedina40degreelook-angle.Thecore ofthecolumnhasacross-sectionalareaof10cm×10cm



Fig.4a,Column12,withsection



Fig.4b,Column12,section,40degree

Fig.4.3-Dreconstructionofcolumn12(experimentalvariant 3)withinstalledmicro-lysimeters.Inthecoreofthe columnthescaledattenuationvaluesfrom0to30are presented.Forabetterview,thesectionwiththelysimetersispresentedina40degreelook-angle.Thecore ofthecolumnhasacross-sectionalareaof10cm×10cm



Figure5a, cross-section of column 1 with microlysimeters (topleft:no2;topright:no3;bottom left:no1;bottom right: no4) and their numbering



Fig.5.Cross-sectionimageofcolumn1withmicro-lysimetersandtheirnumbering(5a)aswellasmicro-lysimeters'respectivemeasuredsamplevolumes(mL),column1(5b)

5c).Micro-lysimeters2and4showidenticalcurves, evenbeforeandafterthebreakincontinuityof leaching.Theirtipslieclosetoeachother(Fig.5a and5b),soweassume,thesesuctionlysimetersshowedr eciprocalinfluence.Modelingofthe breakthroughcurvesdidn'tmakesense.Incolumns5 and12,bothpreviouslydried,atleastonemicrolysimeterhaddirectcontacttoamacropore(Fig.6a, microlysimeterno4andFig.7amicro-lysimeterno 15).Thesemicro-lysimetersshowedthelowestsuction performancewithintheircolumn.Thus,contacttoa macropore(>0.5cm)appearstohaveaclear influenceonthesuctionperformanceofamicro-



Fig.6across-sectionofcolumn5withmicro-lysimeters(top left:no4;topright:no1;bottomleft:no3;bottomright:no2) and their numbering





lysimeter.Underunsaturatedconditions,onlyathin filmofwaterispresentonthewallsofporesofthis diameter.Becauseofthis,thesesuctionlysimeters drainednosolutionmostofthetime,andhencelowvolume ofleachate.Transferringthisresulttonatural conditionswherethemicro-lysimeterswouldrepresent therootingzoneofforesttreesitcanbeassumedthat alreadyunderthesesimulateddroughtconditions waterstresswouldhavebegun.

Micro-lysimetersinacompactsoilmatrixalso showedlowsuctionperformance.Aplacement avoidingtheseextremesresultedinsatisfactoryfunctio ning.Ifenoughfineporesarepresentinthe vicinityofthemicro-lysimeters,thecapillary



Fig.7aCross-sectionofcolumn12withmicro-lysimeters(top left:no14;topright:no15;bottomleft:no13;bottomright: no16)andtheirnumbering



Fig.7bSamplevolumes(ml)ofcolumn12

Fig.7.Cross-sectionimageofcolumn12withmicro-lysimetersandtheirnumbering(7a)aswellasmicro-lysimeters'respectivemeasuredsamplevolumes(mL),column5(7b)

contributionofwateroutweighstheairfilledporosity, andthevolumeoftheleachatecollectedwillbehigher (Fig.8).Themediandailyamountofleachateafter theinitialphaseoftheexperimentisshownonthe abscissa.Ontheordinate,thecontentofthesolidsin thesoilinanellipsoidalregionaroundthetipofthe microlysimeter(ca.12cm³)isshown.Interestingly, thesuctionperformanceofthemicrolysimeterwithhighporevolumewasaspoorasforlysimeter swith almost100% compactsoilaroundit(column3).Most lysimetersshowbestperformancewithmoderately compactsoil.Inadditiontothetotalquantityofporesandsol idvolume,theporesizedistributionandtheir connectivitytotheimmediatevicinityofthelysimeter



Fig.8.Percentagesoilsolidsaroundthelysimeterinrelation tothesuctionperformanceofthelysimeterfor28lysimetersin7columns.Thesoilsolidcontentwasobtained fromtheCTattenuationdata

isimportant.Allthesefactorsappeartoberesponsible fortheotherwiseunexplainedsuctioneffectiveness ofthelysimeters.Eightofthe28lysimetershaveto beconsideredtobeineffective,sincetheydrainless than1mLd⁻¹(Fig.8).About70% oftheinstalled microlysimetersarecapableofdraining,andabout halfofthemaredistinctlyuseful(>3mLd⁻ ¹)underthegivenconditions.

Forthefirsttime,CTanalysiswasabletovisualizea ndrevealcause-effectrelationshipsofmicrolysimeterporecontactsandtheirsuctionability. TheXrayCTimagesofcrosssectionsofthesoil columnsdidnotshownoticeabledisturbanceinsoilstructu reofthecolumnsduetoinstallationofthe microlysimeters(Figs.5a,6aand7a).Incontrastto this,Beckmannetal.(1992)foundnoticeable disturbancesinsoilstructureduetoinstallationofstandardl ysimetercupsinthefield,resultinginan alterationoftheporesystem.Formostofthedried columns(columns5and12;Figs.10and11)the microlysimetershavemissedthemainbreakthrough astheyhadnoinitialsoilcontactbecauseofthedry stateofthesoil,orthefirstfastbreakthroughbypassed them.

$\label{eq:localization} Localization of the micro-lysimeters and its relation to tracer break through curves$

GiventhatnoCDEmodelcouldbefitforthe microlysimeterdata,itsbreakthroughcurvesin relationtoporestructurecanonlybediscussedina qualitativeway.Asexamplesthe3-Dreconstructionsofcolumns1,5and12withinstalledmicr o-

lysimetersarepresented in figures 2,3 and 4, respectively. The break through curves of all micro-

lysimetersareavailableaswellasall3-

Dreconstructionsofthe scannedsoilcolumns.Thebreakthroughsofthe microlysimetersofcolumn1(thewetvariantofthe experiment)alongwiththebreakthroughofthewhole columnarepresented(Fig.9).Inthiscolumn,the maximumvaluesofthemicro-lysimeterbreakthrough curveswerelowerthanthecolumnoutput.Obviously, thereitwasafastbreakthrough,whichbypassedthe microlysimetersandaslowbreakthroughthatwasseizedbythelys imeter.Thesimilarityofthemicrolysimeterbreakthroughsisexplainedbythefactthat all4micro-lysimetersliedclosetoandinfluenced





1 = column output, 1/1, 1/2, 1/3 and 1/4 = micro-lysimeter

Fig.9.Breakthroughcurvesofcolumn1(experimentalvariant 1)inunitsoftheporevolume.C=measuredconcentration,Co=concentrationoftheBrpulses



 $\label{eq:Fig.10.} Fig.10. Break through curves of column 5 (experimental variant 2) in units of the pore volume. C=measured concentration, Co=concentration of the Brpulses$



12 = column output, 12/13, 12/14, 12/15 and 12/16 = micro-lysimeter

 $\label{eq:Fig.11.Breakthroughcurves of column 12 (experimental variant 3) in units of the pore volume. C=measured concentrations Co=concentration of the Br-pulses$

(notshown). Theselysimeters have participated in the fast break through via the coarse pores, *e.g.* column 2(notshown, lysimeters 5 and 7).

Atleastonemicro-lysimeterofcolumn5(Figs. 3,6aand10)hadveryclearcontacttothemiddleof acoarsepore,whichtraversedthroughthesoil column,andwhichpossiblycontributedtothefast transport.Becauseofthedeficientinitialsoilcontact ortoolowsuctioncapacity,thislysimeterdidnot showthefastbreakthrough.Asinglelysimeterofthe drycolumns,lysimeter14ofcolumn12(Figs.4,7a and11),showedanalmostcompletefast breakthrough.Ofallthelysimetersofthiscolumn, thiswasthefirsttoleadtosoilsolutionleaching,and waspresentinthesoilmatrixwithindirectcontactto coarseporespace.Thisconstellation,amixingof indirectcontacttocoarse-porestransportspaceand directcontacttothefine-porematrix,appearstohave thebestpre-conditionforaquickfunctioningofthe lysimeters,aboveall,indriedsoilsubstance.

Poreconnectivity in the columns and their importance for tracer transport

Forabetterunderstandingofthetotaltransport throughthecolumns,thetransportintopsoilandin subsoilwasconsidered.Thesetwowerecharacterized byadifferentsoilstructureandporestructure.The topsoilhadamoreorlessstronglyexpressedcrumb structurewithhighporosity,whereas,theporosityin thesubsoilwaslow,becauseoftheclaycontent. Hence,itsstructurewasstronglyinfluencedbyroots, faunalburrows,andshrinkagecracksthroughdrying, therefore,containsmacropores.Bothsoilregions, accordingtotheirexpressionoftheirmain characteristics,differentlyinfluencedtracertransport inacolumn.

Luo*etal*.(2010)investigatedquantitative relationshipsbetweenmacroporecharacteristicsand twomajorflowandtransportparameters(K_{sat} and λ). Macroporesplayedanimportantrole.Thetraditional CDEmodeledtheBTCswell.Correlationbetween λ of the wholesoilcolumnand K_{sat} valuesoftheB_thorizon(notA)im pliedthatthedispersivitywasmainlycontrolledbythehori zonwiththelowest K_{sat} inthesoilcolumn.Themostuseful macropore

parametersforpredictingflowandtransportunder saturatedconditionsinthestructuredsoilsincluded macroporosity,numberofpaths,hydraulicradiusand macroporeangle.Thepresenceoftraversingpores(notnec essarilymacroporesintheclassicalsense)in thesubsoilinfluencethevelocityandconcentration of the tracer stransport in this part. The reconstruction oftheflowpatternisdifficult, although the parameters are cl earlydefined. This is because of the interplayof allfactors, withinitial and boundary condition as water con tentcanbedifferenteveninasmallspace buthaveagreatinfluence.Further,theproblemexiststhato nlyverticaltransportmechanismwasconsidered.Asis knownfromdye-experiments,the horizontaltransportalsospreadstoagoodextent (GhodratiandJury1990), that is why, the vertically connectedporesdonotleadtopreferentialflow.



 $\label{eq:Fig.12.} Fig.12. Dispersivity of the bim odal approach in relation to pore structure at three differents cales (P1, P2, P4); three values for the respective column. Dispersivity 1=D1/v1=fastbreak through, dispersivity 2=D2/v2=slow break through (Table 2).$ "Bottom" means subsoil of the column; "top" means tops oil and "comp." means complete column.

Inthesameway, Flury*etal*.(1994)reported thatamajorpartofthewaterflowedpastthesoil matrix.Asaresult, an unexpectedly small portion of the soil, possible took part in the transport. Boolt in k and

Bouma (1991) observed discontinuous macropores, so-called internal catchments, which

shouldbeintegratedinwaterflowmodeling.From studiesonsoilstructureusingx-

rayCT, it was reported by Luo*etal*. (2008) that no macropor eswere continuous from the top to the bottom of the soil column, and some macropores became in effective because of air-entrapment. They concluded that

Table2.Resultsofbimodalparameterevaluation.RetardationfactorR=1,coefficientofdispersivity(cm²Day⁻¹),v=averageporewatervelocity(cmDay⁻¹), D_√/v_v=dispersivity(cm),Br=Bromidequantityof theimpulses(mg).

Column	D1/v1 (cm)(cm)(m	D2/v2 ng)	Br
1	9.0	0.18	14.3
2	8.0	0.63	16.0
3	5.7	0.54	15.0
4	14.5	0.3	15.7
5	19.3	0.0	32.4
6	38.1	0.08	34.5
8	16.0	0.34	14.3
10	24.4	0.49	16.4
11	23.1	0.26	16.8
12	12.9	0.81	11.5

macroporenetworkbyitselfcannotsimplybeequated toapreferentialflownetwork.Accordingly,inthe descriptionofflowprocess,aseriesofcomplex processesneedtobeconsidered.

Inordertodescribetherelationshipbetweenthe BTCandthesoilporecharacteristics, weopposedfit parametersoftheCDEandsoilporeindices. As explainedearlier, theindexes(P_1, P_2 and P_4)werecomputedf ortheporestructureofacolumn. P_1 isan indexforporestructureinsmallerscale. The P_4 on theotherhand, isanindexforcoarseporestructure (Fig.1). Therespective indices, P_1, P_2 and P_4 are shown ontheordinate, Ontheabscissa, either the dispersivity of the slow(D_1/v_1)orfast(D_2/v_2) are shown(Fig.12, Table2). The symbol represents the variant of the experiment(dry, wet) and the area of the column the indexappliesto(top=top-soil, bottom=sub-soil, comp.=complete column).

Infigures12b,12dand12f,correspondingfast dispersivity values (D_2/v_2) in relation to indexes for fine (P_1)),middle(P_2),orcoarse(P_4)poreswere presented.Atallthethreescalesthesefiguresshowed anegativerelationshiptodispersivity, which increased withdecreasingaircontent. This relationship was strongerforcoarserporeindexesintopsoil. The transportpathwayappeardtobeshortenedbyhigheraircon tent,whichloweredfastdispersivity.When coarsepores we represent in the columns (P_4) , then withfastbreakthrough, uniform flow was to be expected, without heterogeneity of pathway of water and ch emicalmovement.Nearlylinearlydecreasing linescouldbeobserved(Fig.12f)fortopsoiland wholecolumnindexes. This happened to alesserextentev enwithmorefinelydividedporespace

(Fig.12d). Theslowdispersivity values had a positive relationship to the pore indices for all scales (Fig. 12a, 12c and 12e) and soil areas, which was nearly linear in all scales. With growing pore content the heterogeneity of the pathways increased. Again, this relationship was more apparent intopsoil.

Allresultshavetobeconsideredwithabitof caution,astheCDEfitwasusingamodel,whichfor thedrycolumnsmightbequestionable.Asa mathematicalmodelitreachedplausibledispersivityvalu es,though.Itexplainswhywecouldnotdetect differencesamongthesoilcolumnsjustby visualizing.Itcanbeassumedthatallcolumnsshowed macroporetransport,whichwasnotlinkedto dispersivityofthesub-soils.

Conclusions

The3Dreconstructionoftheporoussystemcan beusedtodiscussthesuctionperformanceof individualmicro-lysimetersandforexplainingthe breakthroughcurvesofmicro-lysimetersAnumeric poreindexrepresentingavolume'sporecontentataspecific scalecanbecomputedfromCTdata,and doeshavearelationtoflowparameters. Thepore indexhasgenerallyanegativelenearrelationshipwith thefastdispersivity, and a positive lenear relationship with the slow dispersivity. These relations suggest that with increasing porosity, the heterogeneity of the pathwaysincreases.WeconcludethattheCTimageslikecr oss-sectionsand3Dre-constructionsprovide aninterestingandquiteuniqueinsightintothesoilporesyst emaftermoderatedrying.Crosssectionsvisualizingtheporecontactofmicrolysimeters' tips may help to interpret soil water monitoring i nabetter way.

References

- Beckmann, T., Kücke, M., Hasenpusch, K. and Altemüller, H.J. (1992) Einbaubedingte Gefügeänderungeninder Bodenzoneumkeramische Saugkerzen. Zeitschriftfür Pfl anzenernährungund Bodenkunde **155**, 247-250.
- Booltink,H.W.G.andBouma,J.(1991)Physicaland morphologicalcharacterizationofby-passflowina wellstructuredclaysoil.*SoilScienceSocietyof AmericaJournal***55**,1249-1254.

Bouma, J. and Wosten, J. H. M. (1979) Flow patterns during extended unsaturated flow in two, undisturbed swelling claysoil with different microstructures. *Soil Science Society of America Journal* **43**, 16-22.

Borges, J.A.R. and Pires, L.F. (2012) Representative elementary area insoil bulk density measurements through gammaray computed tomography. *Soil and Tillage Research* 123, 43-49.

Flury, M., Fluehler, H., Jury, W.A. and Leuenberger, J. (1994) Susceptibility of soil to preferential flow of water: A field study. *WaterResourcesResearch* **30**, 1945-1954.

Gantzer, C.J. and Anderson, S.H. (2002) Computed tomographic measurement of macroporosity inchiseldiskand non-tillage seed beds. *Soiland Tillage Research* **64**, 101-111.

Ghodrati, M.andJury, W.A. (1990) Afieldstudyusing dyestocharacterizepreferential flow of water. *Soil ScienceSociety of America Journal* **54**, 1558-1563.

Grevers, M.C.J., DeJong, E.andArnaud, R.J.St(1989) The characterization of soil macroporosity with CT scanning. *Canadian Journal of Soil Science* **69**, 629-6.

Hainsworth,J.M.andAylmore,L.A.G(1983)Theuseof computerassistedtomographytodeterminespatialdistributionofso ilwatercontent.*AustralianJournal* ofSoilResearch**21**,435-443.

Heijs, A.W.J., Lange, J., deSchoute, J.F. and Bouma, J. (1995) Computed tomography as atool fornondestructive analysis offlow patterns in macroporous clays oils. *Geoderma* **64**, 183-196.

Heijs, A.W.J., Ritsema, C.J. and Dekkar, L.W. (1996) Three dimensional visualization of preferential flow pattern intwosoils. *Geoderma***70**, 101-116.

Kumar,S.,Anderson,S.H.andUdawatta,R.P.(2010) Agroforestryandgrassbufferinfluenceon macroporesmeasuredbycomputedtomographyunder grazedpasturesystems.*SoilScienceSocietyof AmericaJournal***74**,203-212.

Luo, L.F., Lin, H.S. and Halleck, P. (2008) Quantifying soilstructure and preferential flow inintacts oil using Xray computed to mography. *Soil Science Society of America Journal* **72**, 1058-1069. Luo, L.F., Lin, H.S. and Schmidt, J. (2010) Quantitative relationship between soil macropore characteristics and p referential flow and transport. *Soil Science Society of America Journal* **74**, 1929-1937.

Nielsen, D.R. and Biggar, J.W. (1962) Miscible displacement. 3. Theoretical considerations. Soil Science Society of America Proceedings 26, 216-221.

Peyton,R.L.,Haeffner,B.A.,Anderson,S.H.andGantzer, C.J.(1992)ApplyingX-rayCTtomeasuremacropore diametersinundisturbedsoilcores.*Geoderma***53**, 329-340.

Petrovic, A.M., Siebert, J.E. and Rieke, P.E. (1982) Soil bulkdensity analysis in three dimensions by computer tomographics canning. *Soil Science Society of America Journal* **46**, 445-450.

Pierret, A., Capowiez, Y., Belzunces, L.andMoran, C.J. (2002)3Dreconstructionandquantificationof macroporesusingX-raycomputedtomographyand imageanalysis. *Geoderma***106**, 247-271.

Spangenberg, A., Cecchini, G. and Lamersdorf, N. (1997) Analysing the performance of a microsoil solutions amplin gdevice in a laboratory examination and a field experiment. *Plantand Soil* **196**, 59-70.

Spangenberg, A., Nagarajarao, Y. and Hinz, Ch. (2011) Descriptionoftracertransportthroughmoistanddried soilcolumnsusingabimodalCDEapproach. *FreseniusEnvironmentalBulletin***20**, 616-622.

Taina,L.A.,Heck,R.J.andElliot,T.R.(2008)Application ofXraycomputedtomographytosoilscience:A literaturereview.CanadianJournalofSoilScience 88,1-20.

Toride, N., Leij, F.J. and van Genuchten, M. Th. (1995) The CXTFIT code for estimating transport parameters from la boratory or field tracer experiments. U.S. Salinity Laboratory, U.S. Department of Agriculture, Riverside, California Research Report, 137.

vanGenuchten, M. Th. and Alves, J. W. (1982) Analytical solutions on the one-dimensional convetive-dispersive solute transport equation. USD epartment of Agriculture Technical Bulletin, 133-192.

Warner, J.S., Nieber, J.L., Moore, I.D. and Geese, R.A. (1989) Characterizing macropores insoil by computed tomography. *Soil Science Society of America Journal* **53**, 653-660.