

Acknowledgments

My time as a PhD candidate has been a great experience full of important lessons within and beyond my research field. This would not have been possible without the excellent supervision I have received from my supervisor Dr. Boris van Breukelen. Boris, thank you a lot for keeping the right balance between letting me find my way on my own and leading me when I got stuck. Especially in the last year of my PhD, when I ran a bit out of time, you helped me out a lot in a very efficient and constructive way! Your masterstroke of splitting one manuscript into two SISS model papers really turned the tide!

Ilja, thank you for keeping up the female hydrologist power in our group, and for your help with the modeling, especially when some expertise in the setup and parameterization of the hillslope model was called for. Also, your help with scientific writing in English was crucial to (or would it be for?) improving the conciseness of my manuscripts. Maarten, thanks so much for providing our floor with a lot of liveliness, motivation, and coffee, but also for telling me when it was really time to go home.

Ype, thanks a lot for your brilliant work with the pesticide model. I really appreciate that you always took the time to explain the model and discuss results with me. I feel as if I was stealing first authorship from you. Marie, Gwenaël, Sylvain, thanks for your hospitality when I came to Strasbourg, your interest in my work, countless enlightening e-mails, and the willingness to leave one of the most innovative parts of your study to me - the precious CSIA data! I would also like to thank Joachim Rozemeijer and Rob McLaren for their help with HydroGeoSphere.

I am very grateful for all the opportunities the CSI:environment network provided. It was very inspiring to learn from the diverse expertise of all the scientists in the network. And of course I enjoyed the traveling and looking behind the scenes at other institutes. Thanks to the network, I also got to know a very good friend. Tania, thank you so much for all the fun we shared in Europe and elsewhere, and for your help with my Leipzig mission!

My special thanks also go to the members of the reading committee, Dr. Hans Peter Broers, Dr. Martin Elsner, Prof.Dr. Daniel Hunkeler, Prof.Dr. Stefan Uhlenbrook, and Prof.Dr. Sjoerd van der Zee, for the diligent assessment of this thesis.

I am most thankful for the help I got with editing and formatting this book. Vielen, vielen Dank, Doris, für die schnelle und professionelle Gestaltung von einem großartigen Cover! Veelmals bedankt, Anne, voor je hulp met de Nederlandse samenvatting - dat is conversation exchange op zijn best!

Thanks for the company to everyone who has worked with me in the Hydro Copyshop. David, muchas gracias for all the encouragement and confidence in me! I admire your passion for science and unshakable positive thinking. So happy to have you as a friend and cherished pen pal! Jun and Liang, I think we formed the best Eurasian office ever! Thanks for your support and patience in the final phase of my PhD.

Patricia, I thoroughly enjoyed all the dancing you and others brought to our office. Thanks also to Herman who discovered my talent as paranimf.

Mari, you are simply the best! Danke für dein grenzenloses Verständnis und all die Unterstützung, für die tollsten Kaffeepausen, Abendessen, Ausflüge ins Amsterdamer Nachtleben, und unser grandioses Urlaubsabenteuer. Yanjiao, thanks for all the good chats - I would not have made it through all this without your invaluable help and encouragement, and the occasional glass of wine we drank! Héloïse, my closest colleague and dearest friend, thank you so much for countless chats, (iso)top food at your place, adventures and fun nights out! Keep up the honor of us hydrology girls! Brett, cheers for regularly checking whether I have to be rescued from underneath a pile of hydrology papers, and for being the best company to enjoy cultural happenings in Amsterdam.

Alex, Andreas, Angela, Artem, Callum, Diego, Hylke, Katerina, Katrin (wir sehen uns wieder in Leipzig!), Margreet, Marjan, Martin, Lintao, Luca, Michi, Ove, Paolo, Paula, Philip, Wouter, Yvonne, Zaman, I am incredibly thankful for all the support, discussions and good times I had with you at the VU and elsewhere. My deepest gratitude also goes to all friends outside of work, you made Amsterdam an unforgettable and unique experience! I will miss you all.

I am most grateful for the support of my family and friends in Germany. Frank, Ani, Gisela, liebe Eltern, vielen Dank für die bedingungslose Unterstützung und Hilfe. Dank euch hatte ich immer einen Zufluchtsort in Deutschland, an dem ich durchatmen und neue Kraft schöpfen konnte. Darum widme ich euch diese Doktorarbeit.

Bibliography

- Abdul, A. S. *Experimental and Numerical studies of the effect of the capillary fringe on streamflow generation*. PhD thesis, University of Waterloo, 1985.
- Abe, Y. and Hunkeler, D. Does the Rayleigh equation apply to evaluate field isotope data in contaminant hydrogeology? *Environmental Science & Technology*, 40(5):1588–1596, 2006.
- Aeppli, C.; Berg, M.; Cirpka, O. A.; Holliger, C.; Schwarzenbach, R. P., and Hofstetter, T. B. Influence of mass-transfer limitations on carbon isotope fractionation during microbial dechlorination of trichloroethene. *Environmental Science & Technology*, 43(23):8813–8820, 2009.
- Aeppli, C.; Hofstetter, T. B.; Amaral, H. I. F.; Kipfer, R.; Schwarzenbach, R. P., and Berg, M. Quantifying in situ transformation rates of chlorinated ethenes by combining compound-specific stable isotope analysis, groundwater dating, and carbon isotope mass balances. *Environmental Science & Technology*, 44(10):3705–3711, 2010.
- Agricola, I.; Friedrich, T., and Spain, P. G. *Elementary geometry*. American Mathematical Society, Providence, R.I., 2008.
- Al-Khatib, K.; Baumgartner Unland, J.; Olson, B. L. S., and Graham, D. W. Alachlor and metolachlor transformation pattern in corn and soil. *Weed Science*, 50(5):581–586, 2002.
- Albrechtsen, H.-J.; Mills, M. S.; Aamand, J., and Bjerg, P. L. Degradation of herbicides in shallow Danish aquifers: an integrated laboratory and field study. *Pest Management Science*, 57(4):341–350, 2001.
- Alletto, L.; Benoit, P.; Bolognesi, B.; Couffignal, M.; Bergheaud, V.; Dumény, V.; Longueval, C., and Barriuso, E. Sorption and mineralisation of S-metolachlor in soils from fields cultivated with different conservation tillage systems. *Soil and Tillage Research*, 128(0):97–103, 2013.
- Amaral, H. I. F.; Aeppli, C.; Kipfer, R., and Berg, M. Assessing the transformation of chlorinated ethenes in aquifers with limited potential for natural attenuation: Added values of compound-specific carbon isotope analysis and groundwater dating. *Chemosphere*, 85(5):774–781, 2011.
- Andersson, A. A systematic examination of a random sampling strategy for source apportionment calculations. *Science of The Total Environment*, 412-413(0):232–238, 2011.
- Annable, W. K.; Frape, S. K.; Shouakar-Stash, O.; Shanoff, T.; Drimmie, R. J., and Harvey, F. E. ^{37}Cl , ^{15}N , ^{13}C isotopic analysis of common agro-chemicals for identifying non-point source agricultural contaminants. *Applied Geochemistry*, 22(7):1530–1536, 2007.
- Anneser, B.; Einsiedl, F.; Meckenstock, R. U.; Richters, L.; Wisotzky, F., and Griebler, C. High-resolution monitoring of biogeochemical gradients in a tar oil-contaminated aquifer. *Applied Geochemistry*, 23(6):1715–1730, 2008.
- Aravena, R. and Hunkeler, D. Investigating the origin and fate of organic contaminants in groundwater using stable isotope analysis. In *Environmental Isotopes in Biodegradation and Bioremediation*, pages 249–291. CRC Press, 2009.
- Arias-Estévez, M.; López-Periago, E.; Martínez-Carballo, E.; Simal-Gándara, J.; Mejuto, J.-C., and García-Río, L. The mobility and degradation of pesticides in soils and the

- pollution of groundwater resources. *Agriculture, Ecosystems & Environment*, 123(4): 247–260, 2008.
- Atteia, O.; Franceschi, M., and Dupuy, A. Validation of reactive model assumptions with isotope data: Application to the Dover case. *Environmental Science & Technology*, 42(9):3289–3295, 2008.
- Badea, S. L.; Vogt, C.; Weber, S.; Danet, A. F., and Richnow, H. H. Stable isotope fractionation of gamma-hexachlorocyclohexane (lindane) during reductive dechlorination by two strains of sulfate-reducing bacteria. *Environmental Science & Technology*, 43(9): 3155–3161, 2009.
- Battaglin, W. A. and Goolsby, Donald A. Are shifts in herbicide use reflected in concentration changes in midwestern rivers? *Environmental Science & Technology*, 33(17): 2917–2925, 1999.
- Beernaerts, S.; Gerard, M.; Debongnie, P.; Barthelemy, J.-P.; Pussemier, L., and Copin, A. Two years of pesticides monitoring in a Belgian watershed. *International Journal of Environmental Analytical Chemistry*, 83(6):469–480, 2003.
- Benettin, P.; van der Velde, Y.; van der Zee, S. E. A. T. M.; Rinaldo, A., and Botter, G. Chloride circulation in a lowland catchment and the formulation of transport by travel time distributions. *Water Resources Research*, 49(8):4619–4632, 2013.
- Bertuzzo, E.; Thomet, M.; Botter, G., and Rinaldo, A. Catchment-scale herbicides transport: Theory and application. *Advances in Water Resources*, 52(0):232–242, 2013.
- Beven, K. Parameter estimation and predictive uncertainty. In *Rainfall-Runoff Modelling*, pages 231–287. John Wiley & Sons, Ltd, 2012.
- Blessing, M.; Schmidt, T. C.; Dinkel, R., and Haderlein, S. B. Delineation of multiple chlorinated ethene sources in an industrialized area—a forensic field study using compound-specific isotope analysis. *Environmental Science & Technology*, 43(8):2701–2707, 2009.
- Blum, P.; Hunkeler, D.; Weede, M.; Beyer, C.; Grathwohl, P., and Morasch, B. Quantification of biodegradation for o-xylene and naphthalene using first order decay models, michaelis-menten kinetics and stable carbon isotopes. *Journal of Contaminant Hydrology*, 105(3-4):118–130, 2009.
- Botter, G.; Bertuzzo, E., and Rinaldo, A. Transport in the hydrologic response: Travel time distributions, soil moisture dynamics, and the old water paradox. *Water Resources Research*, 46(3):W03514, 2010.
- Bouchard, D.; Hunkeler, D.; Gaganis, P.; Aravena, R.; Höhener, P.; Broholm, M. M., and Kjeldsen, P. Carbon isotope fractionation during diffusion and biodegradation of petroleum hydrocarbons in the unsaturated zone: Field experiment at Vaerløse Airbase, Denmark, and modeling. *Environmental Science & Technology*, 42(2):596–601, 2008.
- Brown, V. A.; McDonnell, J. J.; Burns, D. A., and Kendall, C. The role of event water, a rapid shallow flow component, and catchment size in summer stormflow. *Journal of Hydrology*, 217(3-4):171–190, 1999.
- Brunner, P. and Simmons, C. T. Hydrogeosphere: A fully integrated, physically based hydrological model. *Ground Water*, 50(2):170–176, 2012.
- Burt, T. P. and Pinay, G. Linking hydrology and biogeochemistry in complex landscapes. *Progress in Physical Geography*, 29(3):297–316, 2005.
- Buser, H.-R.; Poiger, T., and Müller, M. D. Changed enantiomer composition of metolachlor in surface water following the introduction of the enantiomerically enriched product to the market. *Environmental Science & Technology*, 34(13):2690–2696, 2000.
- Chen, D. J. Z. and MacQuarrie, K. T. B. Numerical simulation of organic carbon, nitrate,

- and nitrogen isotope behavior during denitrification in a riparian zone. *Journal of Hydrology*, 293(1-4):235–254, 2004.
- Christiansen, J. S.; Thorsen, M.; Clausen, T.; Hansen, S., and Refsgaard, J. C. Modelling of macropore flow and transport processes at catchment scale. *Journal of Hydrology*, 299(1-2):136–158, 2004.
- Cifuentes, L. A. and Eldridge, P. M. *A mass- and isotope-balance model of DOC mixing in estuaries*, volume 43. American Society of Limnology and Oceanography, Waco, TX, ETATS-UNIS, 1998.
- Coplen, T. B. Guidelines and recommended terms for expression of stable-isotope-ratio and gas-ratio measurement results. *Rapid Communications in Mass Spectrometry*, 25(17):2538–2560, 2011.
- Cozzarelli, I. M.; Herman, J. S.; Baedecker, M. J., and Fischer, J. M. Geochemical heterogeneity of a gasoline-contaminated aquifer. *Journal of Contaminant Hydrology*, 40(3):261–284, 1999.
- D’Afonseca, F. M.; Prommer, H.; Finkel, M.; Blum, P., and Grathwohl, P. Modeling the long-term and transient evolution of biogeochemical and isotopic signatures in coal tar-contaminated aquifers. *Water Resources Research*, 47(5):W05518, 2011.
- David, M. B.; Gentry, L. E.; Starks, K. M., and Cooke, R. A. Stream transport of herbicides and metabolites in a tile-drained, agricultural watershed. *Journal of Environmental Quality*, 32(5):1790–1801, 2003.
- Deutsch, B.; Mewes, M.; Liskow, I., and Voss, M. Quantification of diffuse nitrate inputs into a small river system using stable isotopes of oxygen and nitrogen in nitrate. *Organic Geochemistry*, 37(10):1333–1342, 2006.
- Divers, M. T.; Elliott, E. M., and Bain, D. J. Quantification of nitrate sources to an urban stream using dual nitrate isotopes. *Environmental Science & Technology*, 2014.
- Doble, R.; Brunner, P.; McCallum, J., and Cook, P. G. An analysis of river bank slope and unsaturated flow effects on bank storage. *Ground Water*, 50(1):77–86, 2012.
- Donald, D. B.; Cessna, A. J.; Sverko, E., and Glozier, N. E. Pesticides in surface drinking-water supplies of the Northern Great Plains. *Environmental Health Perspectives*, 115(8), 2007.
- Doppler, T.; Camenzuli, L.; Hirzel, G.; Krauss, M.; Lück, A., and Stamm, C. Spatial variability of herbicide mobilisation and transport at catchment scale: insights from a field experiment. *Hydrology and Earth System Sciences*, 16(7), 2012.
- Duffy, C. J. and Lee, D.-H. Base flow response from nonpoint source contamination: Simulated spatial variability in source, structure, and initial condition. *Water Resources Research*, 28(3):905–914, 1992.
- Eberts, S. M.; Braun, C., and Jones, S. Compound-specific isotope analysis: Questioning the origins of a trichloroethene plume. *Environmental Forensics*, 9(1):85–95, 2008.
- Eberts, S. M.; Böhlke, J. K.; Kauffman, L. J., and Jurgens, B. C. Comparison of particle-tracking and lumped-parameter age-distribution models for evaluating vulnerability of production wells to contamination. *Hydrogeology Journal*, 20(2):263–282, 2012.
- Elsayed, O. F.; Maillard, E.; Vuilleumier, S.; Nijenhuis, I.; Richnow, H. H., and Imfeld, G. Using compound-specific isotope analysis to assess the degradation of chloroacetanilide herbicides in lab-scale wetlands. *Chemosphere*, 99(0):89–95, 2014.
- Elsner, M. Stable isotope fractionation to investigate natural transformation mechanisms of organic contaminants: principles, prospects and limitations. *Journal of Environmental Monitoring*, 12(11):2005–2031, 2010.
- Elsner, M.; Jochmann, M. A.; Hofstetter, T. B.; Hunkeler, D.; Bernstein, A.; Schmidt, T. C., and Schimmelmann, A. Current challenges in compound-specific stable isotope

- analysis of environmental organic contaminants. *Analytical and Bioanalytical Chemistry*, 403(9):2471–91, 2012.
- Fausser, P.; Thomsen, M.; Sørensen, P., and Petersen, S. Predicted concentrations for pesticides in drainage dominated catchments. *Water, Air, & Soil Pollution*, 187(1): 149–156, 2008.
- Fenner, K.; Canonica, S.; Wackett, L. P., and Elsner, M. Evaluating pesticide degradation in the environment: Blind spots and emerging opportunities. *Science*, 341(6147):752–758, 2013.
- Fischer, A.; Herklotz, I.; Herrmann, S.; Thullner, M.; Weelink, S. A. B.; Stams, A. J. M.; Schlömann, M.; Richnow, H.-H., and Vogt, C. Combined carbon and hydrogen isotope fractionation investigations for elucidating benzene biodegradation pathways. *Environmental Science & Technology*, 42(12):4356–4363, 2008.
- Flipe, N.; Even, S.; Poulin, M.; Théry, S., and Ledoux, E. Modeling nitrate fluxes at the catchment scale using the integrated tool cawaqs. *Science of The Total Environment*, 375(1-3):69–79, 2007.
- Flury, M. Experimental evidence of transport of pesticides through field soils - a review. *Journal of Environmental Quality*, 25(1):25–45, 1996.
- Gassmann, M.; Stamm, C.; Olsson, O.; Lange, J.; Kümmerer, K., and Weiler, M. Model-based estimation of pesticides and transformation products and their export pathways in a headwater catchment. *Hydrology and Earth System Sciences*, 17(12):5213–5228, 2013.
- Gavrilescu, M. Fate of pesticides in the environment and its bioremediation. *Engineering in life sciences*, 5(6):497–526, 2005.
- Giebel, B. M.; Swart, P. K., and Riemer, D. D. New insights to the use of ethanol in automotive fuels: A stable isotopic tracer for fossil- and bio-fuel combustion inputs to the atmosphere. *Environmental Science & Technology*, 45(15):6661–6669, 2011.
- Ging, P.B.; Lee, R.W., and Silva, S.R. Water chemistry of Shoal Creek and Waller Creek, Austin, Texas, and potential sources of nitrate. Water-Resources Investigations Report 96-4167. Technical report, U.S. Geological Survey, 1996.
- Goderniaux, P.; Brouyère, S.; Fowler, H. J.; Blenkinsop, S.; Therrien, R.; Orban, P., and Dassargues, A. Large scale surface-subsurface hydrological model to assess climate change impacts on groundwater reserves. *Journal of Hydrology*, 373(1-2):122–138, 2009.
- Green, C. T.; Böhlke, J. K.; Bekins, B. A., and Phillips, S. P. Mixing effects on apparent reaction rates and isotope fractionation during denitrification in a heterogeneous aquifer. *Water Resources Research*, 46(8), 2010.
- Griebler, C.; Safinowski, M.; Vieth, A.; Richnow, H. H., and Meckenstock, R. U. Combined application of stable carbon isotope analysis and specific metabolites determination for assessing in situ degradation of aromatic hydrocarbons in a tar oil-contaminated aquifer. *Environmental Science & Technology*, 38(2):617–631, 2004.
- Grube, A.; Donaldson, D.; Kiely, T., and Wu, L. Pesticides industry sales and usage 2006 and 2007 market estimates. Technical report, U.S. Environmental Protection Agency, 2011.
- Gutierrez, A. and Baran, N. Long-term transfer of diffuse pollution at catchment scale: Respective roles of soil, and the unsaturated and saturated zones (Brévilles, France). *Journal of Hydrology*, 369(3-4):381–391, 2009.
- Hartenbach, A. E.; Hofstetter, T. B.; Tentscher, P. R.; Canonica, S.; Berg, M., and Schwarzenbach, R. P. Carbon, hydrogen, and nitrogen isotope fractionation during light-induced transformations of atrazine. *Environmental Science & Technology*, 42(21): 7751–7756, 2008.

- Health & Consumer Protection Directorate, . Review report for the active substance S-metolachlor. Technical report, European Commission, 2004.
- Henderson, K. L.; Belden, J. B., and Coats, J. R. Mass balance of metolachlor in a grassed phytoremediation system. *Environmental Science & Technology*, 41(11):4084–4089, 2007.
- Holvoet, K. M. A.; Seuntjens, P., and Vanrolleghem, P. A. Monitoring and modeling pesticide fate in surface waters at the catchment scale. *Ecological Modelling*, 209(1): 53–64, 2007.
- Hopp, L. and McDonnell, J. J. Connectivity at the hillslope scale: Identifying interactions between storm size, bedrock permeability, slope angle and soil depth. *Journal of Hydrology*, 376(3-4):378–391, 2009.
- Hopp, L. and McDonnell, J. J. Examining the role of throughfall patterns on subsurface stormflow generation. *Journal of Hydrology*, 409(1-2):460–471, 2011.
- Hopp, L.; Harman, C.; Desilets, S. L. E.; Graham, C. B.; McDonnell, J. J., and Troch, P. A. Hillslope hydrology under glass: confronting fundamental questions of soil-water-biota co-evolution at Biosphere 2. *Hydrology and Earth System Sciences*, 13(11):2105 – 2118, 2009.
- Hrachowitz, M.; Savenije, H.; Bogaard, T. A.; Tetzlaff, D., and Soulsby, C. What can flux tracking teach us about water age distribution patterns and their temporal dynamics? *Hydrology and Earth System Sciences*, 17(2):533–564, 2013.
- Hunkeler, D. and Elsner, M. Principles and mechanisms of isotope fractionation. In Marjorie Aelion, C.; Aravena, R.; Hunkeler, D., and Höhener, P., editors, *Environmental Isotopes in Biodegradation and Bioremediation*, pages 43–77. CRC Press, 2009.
- Hunkeler, D.; Aravena, R.; Berry-Spark, K., and Cox, E. Assessment of degradation pathways in an aquifer with mixed chlorinated hydrocarbon contamination using stable isotope analysis. *Environmental Science & Technology*, 39(16):5975–5981, 2005.
- Hunkeler, D.; van Breukelen, B. M., and Elsner, M. Modeling chlorine isotope trends during sequential transformation of chlorinated ethenes. *Environmental Science & Technology*, 43(17):6750–6756, 2009.
- James, A. L.; McDonnell, J. J.; Tromp-van Meerveld, H. J., and Peters, N. E. Gypsies in the palace: experimentalist’s view on the use of 3-D physics-based simulation of hillslope hydrological response. *Hydrological Processes*, 24(26):3878–3893, 2010.
- Jin, B.; Haderlein, S. B., and Rolle, M. Integrated carbon and chlorine isotope modeling: Applications to chlorinated aliphatic hydrocarbons dechlorination. *Environmental Science & Technology*, 47(3):1443–1451, 2013.
- Jochmann, M. A.; Blessing, M.; Haderlein, S. B., and Schmidt, T. C. A new approach to determine method detection limits for compound-specific isotope analysis of volatile organic compounds. *Rapid Communications in Mass Spectrometry*, 20(24):3639–3648, 2006.
- Johannsen, A.; Dähnke, K., and Emeis, K. Isotopic composition of nitrate in five German rivers discharging into the North Sea. *Organic Geochemistry*, 39(12):1678–1689, 2008.
- Joly, P.; Besse-Hoggan, P.; Bonnemoy, F.; Batisson, I.; Bohatier, J., and Mallet, C. Impact of maize formulated herbicides mesotrione and S-metolachlor, applied alone and in mixture, on soil microbial communities. *ISRN Ecology*, 2012:9, 2012.
- Jones, R.L. and Norris, F.A. Factors affecting degradation of aldicarb and ethoprop. *Journal of Nematology*, 30(1):45–55, 1998.
- Kampf, S. K. and Burges, S. J. A framework for classifying and comparing distributed hillslope and catchment hydrologic models. *Water Resources Research*, 43(5), 2007.

- Kawashima, H. and Katayama, Y. Source evaluation of diazinon using stable carbon isotope ratio. *Environmental Forensics*, 11(4):363–371, 2010.
- Kellman, L. M. and Hillaire-Marcel, C. Evaluation of nitrogen isotopes as indicators of nitrate contamination sources in an agricultural watershed. *Agriculture, Ecosystems & Environment*, 95(1):87–102, 2003.
- Kjær, J.; Olsen, P.; Henriksen, T., and Ullum, M. Leaching of metribuzin metabolites and the associated contamination of a sandy Danish aquifer. *Environmental Science & Technology*, 39(21):8374–8381, 2005.
- Kolhatkar, R.; Kuder, T.; Philp, P.; Allen, J., and Wilson, J. T. Use of compound-specific stable carbon isotope analyses to demonstrate anaerobic biodegradation of MTBE in groundwater at a gasoline release site. *Environmental Science & Technology*, 36(23): 5139–5146, 2002.
- Kolpin, D. W.; Thurman, E. M., and Linhart, S. M. The environmental occurrence of herbicides: The importance of degradates in ground water. *Archives of Environmental Contamination and Toxicology*, 35(3):385–390, 1998.
- Konstantinou, I. K.; Zarkadis, A. K., and Albanis, T. A. Photodegradation of selected herbicides in various natural waters and soils under environmental conditions. *Journal of Environmental Quality*, 30(1):121–130, 2001.
- Kopinke, F.-D.; Georgi, A.; Voskamp, M., and Richnow, H. H. Carbon isotope fractionation of organic contaminants due to retardation on humic substances: Implications for natural attenuation studies in aquifers. *Environmental Science & Technology*, 39(16):6052–6062, 2005.
- Kreuger, J. Pesticides in stream water within an agricultural catchment in southern sweden, 1990-1996. *The Science of The Total Environment*, 216(3):227–251, 1998.
- Kronimus, A.; Schwarzbauer, J.; Dsikowitzky, L., and Littke, R. Compound-specific stable carbon isotope analyses of riverine water organic contaminants. *Environmental Chemistry Letters*, 4(1):23–28, 2006.
- Kuder, T.; Wilson, J. T.; Kaiser, P.; Kolhatkar, R.; Philp, P., and Allen, J. Enrichment of stable carbon and hydrogen isotopes during anaerobic biodegradation of MTBE: Microcosm and field evidence. *Environmental Science & Technology*, 39(1):213–220, 2004.
- Le Bot, B.; Oulhote, Y.; Deguen, S., and Glorennec, P. Using and interpreting isotope data for source identification. *TrAC Trends in Analytical Chemistry*, 30(2):302–312, 2011.
- Lee, T. and Benson, C. H. Sorption and degradation of alachlor and metolachlor in ground water using green sands. *Journal of Environmental Quality*, 33(5):1682–1693, 2004.
- Lefranq, M. *Transport and attenuation of pesticides in runoff from agricultural headwater catchments: from field characterisation to modelling*. PhD thesis, Université de Strasbourg, 2014.
- Leu, C.; Singer, H.; Stamm, C.; Müller, S. R., and Schwarzenbach, R. P. Simultaneous assessment of sources, processes, and factors influencing herbicide losses to surface waters in a small agricultural catchment. *Environmental Science & Technology*, 38(14): 3827–3834, 2004a.
- Leu, C.; Singer, H.; Stamm, C.; Müller, S. R., and Schwarzenbach, R. P. Variability of herbicide losses from 13 fields to surface water within a small catchment after a controlled herbicide application. *Environmental Science & Technology*, 38(14):3835–3841, 2004b.
- Li, Q.; Unger, A. J. A.; Sudicky, E. A.; Kassenaar, D.; Wexler, E. J., and Shikaze, S. Simulating the multi-seasonal response of a large-scale watershed with a 3D physically-based hydrologic model. *Journal of Hydrology*, 357(3-4):317–336, 2008.

- Liu, K.; Cao, Z.; Pan, X., and Yu, Y. Using in situ pore water concentrations to estimate the phytotoxicity of nicosulfuron in soils to corn (*Zea mays* L.). *Environmental Toxicology and Chemistry*, 31(8):1705–11, 2012.
- Liu, T.; Wang, F.; Michalski, G.; Xia, X., and Liu, S. Using ^{15}N , ^{17}O , and ^{18}O to determine nitrate sources in the Yellow River, China. *Environmental Science & Technology*, 47(23):13412–13421, 2013.
- Louchart, X.; Voltz, M.; Andrieux, P., and Moussa, R. Herbicide transport to surface waters at field and watershed scales in a Mediterranean vineyard area. *Journal of Environmental Quality*, 30(3):982–991, 2001.
- Mancini, S. A.; Lacrampe-Couloume, G.; Jonker, H.; van Breukelen, B. M.; Groen, J.; Volkering, F., and Sherwood Lollar, B. Hydrogen isotopic enrichment: An indicator of biodegradation at a petroleum hydrocarbon contaminated field site. *Environmental Science & Technology*, 36(11):2464–2470, 2002.
- Mancini, S. A.; Ulrich, A. C.; Lacrampe-Couloume, G.; Sleep, B.; Edwards, E. A., and Sherwood Lollar, B. Carbon and hydrogen isotopic fractionation during anaerobic biodegradation of benzene. *Applied and Environmental Microbiology*, 69(1):191–198, 2003.
- Mancini, S. A.; Lacrampe-Couloume, G., and Lollar, B. S. Source differentiation for benzene and chlorobenzene groundwater contamination: A field application of stable carbon and hydrogen isotope analyses. *Environmental Forensics*, 9(2-3):177–186, 2008.
- Mariotti, A.; Germon, J. C.; Hubert, P.; Kaiser, P.; Letolle, R.; Tardieux, A., and Tardieux, P. Experimental determination of nitrogen kinetic isotope fractionation: Some principles; illustration for the denitrification and nitrification processes. *Plant and Soil*, 62(3): 413–430, 1981.
- McCallum, J. L.; Cook, P. G.; Brunner, P., and Berhane, D. Solute dynamics during bank storage flows and implications for chemical base flow separation. *Water Resources Research*, 46(7):W07541, 2010.
- Meckenstock, R. U.; Morasch, B.; Griebler, C., and Richnow, H. H. Stable isotope fractionation analysis as a tool to monitor biodegradation in contaminated aquifers. *Journal of Contaminant Hydrology*, 75(3-4):215–255, 2004.
- Meyer, A. H. and Elsner, M. $^{13}\text{C}/^{12}\text{C}$ and $^{15}\text{N}/^{14}\text{N}$ isotope analysis to characterize degradation of atrazine: Evidence from parent and daughter compound values. *Environmental Science & Technology*, 47(13):6884–6891, 2013.
- Meyer, A. H.; Penning, H.; Lowag, H., and Elsner, M. Precise and accurate compound specific carbon and nitrogen isotope analysis of atrazine: Critical role of combustion oven conditions. *Environmental Science & Technology*, 42(21):7757–7763, 2008.
- Meyer, A. H.; Penning, H., and Elsner, M. C and N isotope fractionation suggests similar mechanisms of microbial atrazine transformation despite involvement of different enzymes (AtzA and TrzN). *Environmental Science & Technology*, 43(21):8079–8085, 2009.
- Milosevic, N.; Qiu, S.; Elsner, M.; Einsiedl, F.; Maier, M. P.; Bensch, H. K. V.; Albrechtsen, H. J., and Bjerg, P. L. Combined isotope and enantiomer analysis to assess the fate of phenoxy acids in a heterogeneous geologic setting at an old landfill. *Water Research*, 47(2):637–649, 2013.
- Mirus, B. B. and Loague, K. How runoff begins (and ends): Characterizing hydrologic response at the catchment scale. *Water Resources Research*, 49(5):2987–3006, 2013.
- Mirus, B. B.; Ebel, B. A.; Heppner, C. S., and Loague, K. Assessing the detail needed to capture rainfall-runoff dynamics with physics-based hydrologic response simulation. *Water Resources Research*, 47(3):1944–1973, 2011.

- Moore, J. W. and Semmens, B. X. Incorporating uncertainty and prior information into stable isotope mixing models. *Ecology Letters*, 11(5):470–480, 2008.
- Morasch, B.; Hunkeler, D.; Zopfi, J.; Temime, B., and Höhener, P. Intrinsic biodegradation potential of aromatic hydrocarbons in an alluvial aquifer – potentials and limits of signature metabolite analysis and two stable isotope-based techniques. *Water Research*, 45(15):4459–4469, 2011.
- Müller, K.; Bach, M.; Hartmann, H.; Spiteller, M., and Frede, H. G. Point- and nonpoint-source pesticide contamination in the Zwesten Ohm catchment, Germany. *Journal of Environmental Quality*, 31(1):309–18, 2002.
- Müller, K.; Deurer, M.; Hartmann, H.; Bach, M.; Spiteller, M., and Frede, H. G. Hydrological characterisation of pesticide loads using hydrograph separation at different scales in a German catchment. *Journal of Hydrology*, 273(1-4):1–17, 2003.
- Okuda, T.; Kumata, H.; Zakaria, M. P.; Naraoka, H.; Ishiwatari, R., and Takada, H. Source identification of Malaysian atmospheric polycyclic aromatic hydrocarbons nearby forest fires using molecular and isotopic compositions. *Atmospheric Environment*, 36(4): 611–618, 2002.
- Otto, R. Estimating groundwater recharge rates in the southeastern Holstein region, northern Germany. *Hydrogeology Journal*, 9(5):498–511, 2001.
- Overeem, A.; Buishand, T. A., and Holleman, I. Extreme rainfall analysis and estimation of depth-duration-frequency curves using weather radar. *Water Resources Research*, 45(10):W10424, 2009.
- Parkhurst, D. L.; Kipp, K. L., and Charlton, S. R. PHAST version 2–A program for simulating groundwater flow, solute transport, and multicomponent geochemical reactions. Technical report, U.S. Geological Survey Techniques and Methods 6-A35, 2010.
- Parochetti, J. V. Photodecomposition, volatility and leaching of atrazine, simazine, alachlor and metolachlor from soil and plant material. Weed Science Society of America, abstract no. 17, 1978.
- Payraudeau, S. and Gregoire, C. Modelling pesticides transfer to surface water at the catchment scale: a multi-criteria analysis. *Agronomy for Sustainable Development*, 32(2):479–500, 2012.
- Penning, H. and Elsner, M. Intramolecular carbon and nitrogen isotope analysis by quantitative dry fragmentation of the phenylurea herbicide isoproturon in a combined injector/capillary reactor prior to GC separation. *Analytical Chemistry*, 79(21):8399–8405, 2007.
- Penning, H.; Sørensen, S. R.; Meyer, A. H.; Aamand, J., and Elsner, M. C, N, and H isotope fractionation of the herbicide isoproturon reflects different microbial transformation pathways. *Environmental Science & Technology*, 44(7):2372–2378, 2010.
- Phillips, D. and Gregg, J. Uncertainty in source partitioning using stable isotopes. *Oecologia*, 127:171–179, 2001.
- Phillips, D. and Koch, P. Incorporating concentration dependence in stable isotope mixing models. *Oecologia*, 130:114–125, 2002.
- Pooley, K. E.; Blessing, M.; Schmidt, T. C.; Haderlein, S. B.; Macquarrie, K. T. B., and Prommer, H. Aerobic biodegradation of chlorinated ethenes in a fractured bedrock aquifer: Quantitative assessment by compound-specific isotope analysis (CSIA) and reactive transport modeling. *Environmental Science & Technology*, 43(19):7458–7464, 2009.
- Prommer, H.; Anneser, B.; Rolle, M.; Einsiedl, F., and Griebler, C. Biogeochemical and isotopic gradients in a BTEX/PAH contaminant plume: Model-based interpretation of

- a high-resolution field data set. *Environmental Science & Technology*, 43(21):8206–8212, 2009.
- Qiu, S.; Eckert, D.; Cirpka, O. A.; Huenniger, M.; Knappett, P.; Maloszewski, P.; Meckenstock, R. U.; Griebler, C., and Elsner, M. Direct experimental evidence of non-first order degradation kinetics and sorption-induced isotopic fractionation in a mesoscale aquifer: $^{13}\text{C}/^{12}\text{C}$ analysis of a transient toluene pulse. *Environmental Science & Technology*, 47(13):6892–6899, 2013.
- Querner, E. P. The effects of human intervention in the water regime. *Ground Water*, 38(2):167–171, 2000.
- Quilbe, R.; Rousseau, A. N.; Lafrance, P.; Leclerc, J., and Amrani, M. Selecting a pesticide fate model at the watershed scale using a multi-criteria analysis. *Water Quality Research Journal of Canada*, 41(3):283–295, 2006.
- Rabiet, M.; Margoum, C.; Gouy, V.; Carluier, N., and Coquery, M. Assessing pesticide concentrations and fluxes in the stream of a small vineyard catchment – effect of sampling frequency. *Environmental Pollution*, 158(3):737–748, 2010.
- Rawn, D F. K. and Muir, Derek C. G. Sources of chlorpyrifos and dacthal to a small Canadian prairie watershed. *Environmental Science & Technology*, 33(19):3317–3323, 1999.
- Reinnicke, S; Simonsen, A; Sørensen, S R.; Aamand, J, and Elsner, M. C and N isotope fractionation during biodegradation of the pesticide metabolite 2,6-dichlorobenzamide (BAM): Potential for environmental assessments. *Environmental Science & Technology*, 46(3):1447–1454, 2011.
- Rice, P. J.; Anderson, T. A., and Coats, J. R. Degradation and persistence of metolachlor in soil: Effects of concentration, soil moisture, soil depth, and sterilization. *Environmental Toxicology and Chemistry*, 21(12):2640–2648, 2002.
- Richards, R. P. and Baker, D. B. Pesticide concentration patterns in agricultural drainage networks in the lake erie basin. *Environmental Toxicology and Chemistry*, 12(1):13–26, 1993.
- Rivard, L. Environmental fate of metolachlor, 2003.
- Rivett, M. O.; Chapman, S. W.; Allen-King, R. M.; Feenstra, S., and Cherry, J. A. Pump-and-treat remediation of chlorinated solvent contamination at a controlled field-experiment site. *Environmental Science & Technology*, 40(21):6770–6781, 2006.
- Rodríguez-Cruz, M. S.; Jones, J. E., and Bending, G. D. Field-scale study of the variability in pesticide biodegradation with soil depth and its relationship with soil characteristics. *Soil Biology and Biochemistry*, 38(9):2910–2918, 2006.
- Rolle, M.; Chiogna, G.; Bauer, R.; Griebler, C., and Grathwohl, P. Isotopic fractionation by transverse dispersion: Flow-through microcosms and reactive transport modeling study. *Environmental Science & Technology*, 44(16):6167–6173, 2010.
- Rozemeijer, J. C. and Broers, H. P. The groundwater contribution to surface water contamination in a region with intensive agricultural land use (Noord-Brabant, The Netherlands). *Environmental Pollution*, 148(3):695–706, 2007.
- Schmidt, T. C. and Jochmann, M. A. Origin and fate of organic compounds in water: characterization by compound-specific stable isotope analysis. *Annual Review of Analytical Chemistry*, 5:133–55, 2012.
- Schmidt, T. C.; Zwank, L.; Elsner, M.; Berg, M.; Meckenstock, R. U., and Haderlein, S. B. Compound-specific stable isotope analysis of organic contaminants in natural environments: a critical review of the state of the art, prospects, and future challenges. *Analytical and Bioanalytical Chemistry*, 378(2):283–300, 2004.

- Schreglmann, K.; Hoeche, M.; Steinbeiss, S.; Reinicke, S., and Elsner, M. Carbon and nitrogen isotope analysis of atrazine and desethylatrazine at sub-microgram per liter concentrations in groundwater. *Analytical and Bioanalytical Chemistry*, 405(9): 2857–2867, 2013.
- Seiler, R. L. Combined use of ^{15}N and ^{18}O of nitrate and ^{11}B to evaluate nitrate contamination in groundwater. *Applied Geochemistry*, 20(9):1626–1636, 2005.
- Sherwood Lollar, B.; Slater, G. F.; Sleep, B.; Witt, M.; Klecka, G. M.; Harkness, M., and Spivack, J. Stable carbon isotope evidence for intrinsic bioremediation of tetrachloroethene and trichloroethene at area 6, Dover Air Force Base. *Environmental Science & Technology*, 35(2):261–9, 2001.
- Sherwood Lollar, B.; Hirschorn, S. K.; Chartrand, M. M. G., and Lacrampe-Couloume, G. An approach for assessing total instrumental uncertainty in compound-specific carbon isotope analysis: Implications for environmental remediation studies. *Analytical Chemistry*, 79(9):3469–3475, 2007.
- Si, Y.; Takagi, K.; Iwasaki, A., and Zhou, D. Adsorption, desorption and dissipation of metolachlor in surface and subsurface soils. *Pest Management Science*, 65(9):956–962, 2009.
- Squillace, P. J. and Thurman, E. M. Herbicide transport in rivers: Importance of hydrology and geochemistry in nonpoint-source contamination. *Environmental Science and Technology*, 26:538–545, 1992.
- Sturchio, N. C.; Böhlke, J. K.; Gu, B.; Horita, J.; Brown, G. M.; Beloso, A. D. Jr.; Patterson, L. J.; Hatzinger, P. B.; Jackson, W. A., and Batista, J. Stable isotopic composition of chlorine and oxygen in synthetic and natural perchlorate. In Baohua, G. and Coates, J. D., editors, *Perchlorate*, pages 93–109. Springer US, 2006.
- Sturchio, N. C.; Böhlke, J. K.; Beloso, A. D.; Streger, S. H.; Heraty, L. J., and Hatzinger, P. B. Oxygen and chlorine isotopic fractionation during perchlorate biodegradation: Laboratory results and implications for forensics and natural attenuation studies. *Environmental Science & Technology*, 41(8):2796–2802, 2007.
- Sturchio, N. C.; Hoaglund, J. R.; Marroquin, R. J.; Beloso, A. D.; Heraty, L. J.; Bortz, S. E., and Patterson, T. L. Isotopic mapping of groundwater perchlorate plumes. *Ground Water*, 50(1):94–102, 2012.
- Sudicky, E. A.; Illman, W. A.; Goltz, I. K.; Adams, J. J., and McLaren, R. G. Heterogeneity in hydraulic conductivity and its role on the macroscale transport of a solute plume: From measurements to a practical application of stochastic flow and transport theory. *Water Resources Research*, 46(1):W01508, 2010.
- Taghavi, L.; Merlina, G., and Probst, J.-L. The role of storm flows in concentration of pesticides associated with particulate and dissolved fractions as a threat to aquatic ecosystems - case study: the agricultural watershed of Save river (Southwest of France). *Knowledge and Management of Aquatic Ecosystems*, (400):06, 2011.
- Therrien, R.; McLaren, R. G.; Sudicky, E. A., and Panday, S. M. HydroGeoSphere, a three-dimensional numerical model describing fully integrated subsurface and surface flow and solute transport, draft. Technical report, Groundwater Simulation Group, University of Waterloo, 2010.
- Thompson, A.; Rudolph, J.; Rohrer, F., and Stein, O. Concentration and stable carbon isotopic composition of ethane and benzene using a global three-dimensional isotope inclusive chemical tracer model. *Journal of Geophysical Research: Atmospheres*, 108 (D13):4373, 2003.
- Thorsen, M.; Feyen, J., and Styczen, M. Agrochemical modelling. In Abbott, M.B. and Refsgaard, J.C., editors, *Distributed Hydrological Modelling*, pages 121–141. Kluwer Academic Publishers, Dordrecht, The Netherlands, 1996.

- Thullner, M.; Centler, F.; Richnow, H.-H., and Fischer, A. Quantification of organic pollutant degradation in contaminated aquifers using compound specific stable isotope analysis - review of recent developments. *Organic Geochemistry*, 42(12):1440–1460, 2012.
- University of Hertfordshire, The Pesticide Properties DataBase (PPDB) developed by the Agriculture & Environment Research Unit (AERU), University of Hertfordshire, 2013.
- van Breukelen, B. M. Extending the Rayleigh equation to allow competing isotope fractionating pathways to improve quantification of biodegradation. *Environmental Science & Technology*, 41(11):4004–4010, 2007a.
- van Breukelen, B. M. Quantifying the degradation and dilution contribution to natural attenuation of contaminants by means of an open system Rayleigh equation. *Environmental Science & Technology*, 41(14):4980–4985, 2007b.
- van Breukelen, B. M. and Prommer, H. Beyond the Rayleigh equation: Reactive transport modeling of isotope fractionation effects to improve quantification of biodegradation. *Environmental Science & Technology*, 42(7):2457–2463, 2008.
- van Breukelen, B. M. and Rolle, M. Transverse hydrodynamic dispersion effects on isotope signals in groundwater chlorinated solvents' plumes. *Environmental Science & Technology*, 46(14):7700–7708, 2012.
- van Breukelen, B. M.; Hunkeler, D., and Volkering, F. Quantification of sequential chlorinated ethene degradation by use of a reactive transport model incorporating isotope fractionation. *Environmental Science & Technology*, 39(11):4189–4197, 2005.
- van den Berg, F.; Kubiak, R.; Benjey, W. G.; Majewski, M. S.; Yates, S. R.; Reeves, G. L.; Smelt, J. H., and van der Linden, A. M. A. Emission of pesticides into the air. *Water, Air, & Soil Pollution*, 115(1):195–218, 1999.
- van der Velde, Y.; de Rooij, G. H.; Rozemeijer, J. C.; van Geer, F. C., and Broers, H. P. Nitrate response of a lowland catchment: On the relation between stream concentration and travel time distribution dynamics. *Water Resources Research*, 46(11):W11534, 2010.
- van der Velde, Y.; Torfs, P. J. J. F.; van der Zee, S. E. A. T. M., and Uijlenhoet, R. Quantifying catchment-scale mixing and its effect on time-varying travel time distributions. *Water Resources Research*, 48(6):W06536, 2012.
- van der Velde, Y.; Heidbüchel, I.; Lyon, S. W.; Nyberg, L.; Rodhe, A.; Bishop, K., and Troch, P. A. Consequences of mixing assumptions for time-variable travel time distributions. Accepted by *Hydrological Processes*, DOI: 10.1002/hyp.10372, 2014.
- van Keer, I.; Bronders, J.; Verhack, J.; Schwarzbauer, J., and Swennen, R. Limitations in the use of compound-specific stable isotope analysis to understand the behaviour of a complex BTEX groundwater contamination near Brussels (Belgium). *Environmental Earth Sciences*, 66(2):457–470, 2012.
- Verbist, K. M. J.; Pierreux, S.; Cornelis, W. M.; McLaren, R., and Gabriels, D. Parameterizing a coupled surface-subsurface three-dimensional soil hydrological model to evaluate the efficiency of a runoff water harvesting technique. *Vadose Zone Journal*, 11(4), 2012.
- Vieth, A.; Kästner, M.; Schirmer, M.; Weiß, H.; Gödeke, S.; Meckenstock, R. U., and Richnow, H. H. Monitoring in situ biodegradation of benzene and toluene by stable carbon isotope fractionation. *Environmental Toxicology and Chemistry*, 24(1):51–60, 2005.
- Voss, M.; Deutsch, B.; Elmgren, R.; Humborg, C.; Kuuppo, P.; Pastuszak, M.; Rolff, C., and Schulte, U. Source identification of nitrate by means of isotopic tracers in the Baltic Sea catchments. *Biogeosciences*, 3(4):663–676, 2006.

- Wang, Y.; Huang, Y. S.; Huckins, J. N., and Petty, J. D. Compound-specific carbon and hydrogen isotope analysis of sub-parts per billion level waterborne petroleum hydrocarbons. *Environmental Science & Technology*, 38(13):3689–3697, 2004.
- Wanner, C.; Eggenberger, U.; Kurz, D.; Zink, S., and Mäder, U. A chromate-contaminated site in southern Switzerland—Part 1: Site characterization and the use of Cr isotopes to delineate fate and transport. *Applied Geochemistry*, 27(3):644–654, 2012a.
- Wanner, C.; Eggenberger, U., and Mäder, U. A chromate-contaminated site in southern Switzerland—Part 2: Reactive transport modeling to optimize remediation options. *Applied Geochemistry*, 27(3):655–662, 2012b.
- Weiler, M. and McDonnell, J. Virtual experiments: a new approach for improving process conceptualization in hillslope hydrology. *Journal of Hydrology*, 285(1-4):3–18, 2004.
- Weller, P.; Boner, M.; Foerstel, H.; Becker, H.; Peikert, B., and Dreher, W. Isotopic fingerprinting for the authenticity control of crop protection active compounds using the representative insecticide fipronil. *Journal of Agricultural and Food Chemistry*, 59(9):4365–4370, 2011.
- Wiegert, C.; Aeppli, C.; Knowles, T.; Holmstrand, H.; Evershed, R.; Pancost, R. D.; Macháčková, J., and Gustafsson, Ö. Dual carbon-chlorine stable isotope investigation of sources and fate of chlorinated ethenes in contaminated groundwater. *Environmental Science & Technology*, 46(20):10918–10925, 2012.
- Wijker, R. S.; Adamczyk, P.; Bolotin, J.; Paneth, P., and Hofstetter, T. B. Isotopic analysis of oxidative pollutant degradation pathways exhibiting large H isotope fractionation. *Environmental Science & Technology*, 47(23):13459–13468, 2013.
- Wriedt, G.; Spindler, J.; Neef, T.; Meißner, R., and Rode, M. Groundwater dynamics and channel activity as major controls of in-stream nitrate concentrations in a lowland catchment system? *Journal of Hydrology*, 343(3-4):154–168, 2007.
- Wu, L.; Yao, J.; Trebse, P.; Zhang, N., and Richnow, H. H. Compound specific isotope analysis of organophosphorus pesticides. *Chemosphere*, 111(0):458–463, 2014.
- Wu, Q.; Riise, G.; Lundekvam, H.; Mulder, J., and Haugen, L. E. Influences of suspended particles on the runoff of pesticides from an agricultural field at Askim, SE-Norway. *Environmental Geochemistry and Health*, 26(2):295–302, 2004.
- Xue, D.; Botte, J.; De Baets, B.; Accoe, F.; Nestler, A.; Taylor, P.; van Cleemput, O.; Berglund, M., and Boeckx, P. Present limitations and future prospects of stable isotope methods for nitrate source identification in surface- and groundwater. *Water Research*, 43(5):1159–1170, 2009.
- Zehe, E.; Maurer, T.; Ihringer, J., and Plate, E. Modeling water flow and mass transport in a loess catchment. *Physics and Chemistry of the Earth Part B-Hydrology Oceans and Atmosphere*, 26(7-8):487–507, 2001.
- Zhang, Y.-C.; Slomp, C. P.; Broers, H. P.; Bostick, B.; Passier, H. F.; Böttcher, M. E.; Omoregie, E. O.; Lloyd, J. R.; Polya, D. A., and van Cappellen, P. Isotopic and microbiological signatures of pyrite-driven denitrification in a sandy aquifer. *Chemical Geology*, 300-301(0):123–132, 2012.
- Zwank, L.; Berg, M.; Schmidt, T. C., and Haderlein, S. B. Compound-specific carbon isotope analysis of volatile organic compounds in the low-microgram per liter range. *Analytical Chemistry*, 75(20):5575–5583, 2003.
- Zwank, L.; Berg, M.; Elsner, M.; Schmidt, T. C.; Schwarzenbach, R. P., and Haderlein, S. B. New evaluation scheme for two-dimensional isotope analysis to decipher biodegradation processes: Application to groundwater contamination by mtbe. *Environmental Science & Technology*, 39(4):1018–1029, 2005.