To: Dr. Nicholas Woodward
 Department of Energy
 Office of Science SC-64
 19901 Germantown Rd
 Germantown MD 20874-1290
 phone 301-903-5802
 Nick.Woodward@science.doe.gov

*Final Report for Project
 DE-FG02-00ER 15032*

**SIGNIFICANCE OF ISOTOPICALLY LABILE ORGANIC HYDROGEN
 IN THERMAL MATURATION OF ORGANIC MATTER**

Arndt Schimmelmann¹ and Maria Mastalerz²

¹Department of Geological Sciences and ²Indiana Geological Survey

Indiana University, Bloomington IN 47405-1405

aschimme@indiana.edu; phone 812-855-7645

mmastale@indiana.edu; phone 812-855-9416

1. Project Objectives: Explore geochemical conditions and mechanisms that contribute to changes in hydrogen and nitrogen stable isotope ratios in sedimentary organic matter during thermal maturation. Evaluate the diagenetic and/or paleoenvironmental significance of D/H ratios (i.e., ²H/¹H, expressed as customary δD values) in different types of kerogen, macerals, isolates, oils, fractions of oil, and gas.

2. Project Description: Isotopically labile organic hydrogen in fossil fuels occupies chemical positions that participate in isotopic exchange and in chemical reactions during thermal maturation from kerogen to bitumen, oil and gas. Carbon-bound organic hydrogen is isotopically far less exchangeable than hydrogen bound to nitrogen, oxygen, or sulfur. We explore why organic hydrogen isotope ratios express a relationship with organic nitrogen isotope ratios in kerogen at low to moderate maturity. We develop and apply new techniques to utilize organic D/H ratios in organic matter fractions and on a molecular level as tools for exploration for fossil fuels and for paleoenvironmental research. The scope of our samples includes naturally and artificially matured substrates, such as coal, shale, oil and gas.

3. Introduction: Since the beginning of the project in 2000, our research group has enjoyed nine years of valuable DOE financial support and a tenth year of no-cost extension. As of March 2010, our DOE project has resulted in **43 papers** (i.e. 38 published or in press, 5 submitted; all but one have been subject to peer-review) and **67 abstracts** (see listing of all publications with available electronic links below).

We are proud that our DOE-sponsored research provided much exposure and recognition at international and national conferences and professional meetings. Both PIs Schimmelmann and Mastalerz have been **invited keynote speakers** at international meetings (e.g., at the Gordon Conference on Organic Geochemistry in 2007, and at the 2009 ISOCOMPOUND conference). In the past five years, the widespread recognition of our accomplishments resulted in several **invitations to write review articles**, for example in the prestigious *“Annual Review of Earth and Planetary Sciences*;

<http://dx.doi.org/10.1146/annurev.earth.34.031405.125011>), in the “*Encyclopedia of Mass Spectrometry*”, and most recently a chapter for a textbook on coalbed gas. In 2008 Mastalerz received the *Geological Society of America Gilbert H. Cady Award, GSA Coal Geology Division*, “in recognition of distinguished contributions to coal geology”, and in 2009 she was awarded a *Geological Society of America Fellowship*. In 2004 Mastalerz received the *Organic Petrology Award* presented by *International Committee for Coal and Organic Petrology* - in recognition of outstanding contributions to organic petrology and leadership in promoting the development and applying innovative methodologies to the study of coal. Schimmelmann was invited to give presentations about hydrogen stable isotopes in fossil fuels for international oil companies, e.g. *Shell* in the Netherlands and at *ExxonMobil* in Houston, Texas.

DOE funding allowed our group to expand and to rapidly respond to emerging research challenges. Research assistantships and coverage of student travel to conferences provided outstanding benefits for our students and limited their reliance on time-consuming teaching assistantships. During the ten years of DOE support, **four Ph.D. and one master student graduated** from our group. Each one of these graduates served as the first author of one to five peer-reviewed publications, in addition to numerous co-authorships. Our students’ strong publication records contributed to their success in industry and academia (e.g., ExxonMobil, ConocoPhillips, Colorado School of Mines, University of Bristol). In more recent years, our successful research attracted two additional Ph.D. students and one master student who currently remain with us.

During the past six years, our DOE funding and subsequently increased scientific productivity had the pivotal side effect that we were able to attract NSF funding for purchases of a new stable isotope mass spectrometer (Delta Plus XP), a new gas chromatograph-mass spectrometer (Varian 4000 GCMS), and received other funding for a new Fourier-Transform-Infra-Red (FTIR) spectrometer and a new gas chromatograph (SRI Gas Analyzer #2).

4. Summary of selected accomplishments

The following pages briefly describe some of our main accomplishments and cite resulting publications (a complete listing of publications is provided at the end; clicking on the DOI electronic links will make abstracts and in some cases full pdfs available). Our collective work over the years not only addressed questions of our original research proposal, but additionally provided information and preliminary data for new hypotheses about fossil organic matter transformations beyond the scope of our original DOE proposal.

4.1. The isotopic relationship between hydrogen and nitrogen in kerogen as a function of thermal maturity

One aspect of our DOE-funded research project targeted the evaluation of a correlation between the abundance of isotopically exchangeable hydrogen and nitrogen stable isotope ratios (i.e. $\delta^{15}\text{N}$ values) in stratigraphic sequences of kerogens in source rocks. We observed the relationship in thermally immature sequences (e.g., see pdf: [Schimmelmann et al., 2001](#)), but not in thermally more mature ones. The reason was clarified in parallel sets of experiments and publications. First, we collaborated with Jean-Paul Boudou at CNRS Paris/France in an XPS spectroscopic study of organic nitrogen chemistry during low-grade metamorphism. Our data showed that a large portion of organic nitrogen in lower-maturity rocks is linked to organic hydrogen that is isotopically exchangeable. However, with increasing maturity, the shrinking pool of organic nitrogen becomes almost exclusively linked to carbon without exchangeable hydrogen, and thus **$\delta^{15}\text{N}$ loses its relationship with hydrogen exchangeability during low-grade metamorphism**. Our paper was published in *Geochimica et Cosmochimica Acta* ([Boudou et al., 2008](#)). Second, laboratory nitrogen isotope exchange experiments and observations from sedimentary nitrogen phases in the field proved that some of the organic N in kerogen derives from allochthonous mobile and chemically reactive N species (e.g., ammonium, HCN, and low-molecular organic N-containing compounds) that are delivered by migrating fluids to stationary kerogen. N-isotopic exchange between kerogen and NH_4^+ or NH_3 is evident

from experiments where ^{15}N -enriched ammonium chloride solutions and source rocks containing kerogen types I, II, IIS, and III were heated over 5 years at temperatures of 100, 144, and 196°C. The resulting data corroborate our earlier results from our hydrous pyrolysis experiments (330°C for up to 144 hours) and prove that ammonium is readily converted abiogenically to organic N in kerogen at temperatures that approach those in naturally maturing sediments. The propensity of different types of kerogen to react with NH_4^+ or NH_3 increases in the order $\text{II} < \text{I} < \text{IIS} < \text{III}$. Ammonium ions' mobility in formation fluids and their ability to isotopically interact with kerogen makes them an effective isotopic buffer for sedimentary organic N. **Isotopic exchange tends to (i) homogenize the isotopic compositions of participating pools of N, (ii) limits the isotopic ranges of organic and inorganic N, and (iii) consequently decouples $\delta^{15}\text{N}$ from δD .** Recognition of N-exchange in thermally matured sediments offers fresh perspectives and opportunities to constrain the extent and pathways of N-containing geofluid migration, especially when synoptically characterizing organic and mineral-bound N moieties across gradients of thermal maturity. Our results were recently published in *Organic Geochemistry* ([Schimmelmann and Lis, 2010](#)).

4.2. D/H isotopic correlation among formation waters, oil, oil fractions, biomarkers, and kerogen from source rocks

This subproject examined the processes that influence D/H ratios of petroleum and individual biomarkers in Australian oils. We published our paper in *Organic Geochemistry* ([Schimmelmann et al., 2004](#)). D/H ratios of bulk oils, saturated, aromatic, and polar fractions, individual *n*-alkanes, formation waters and non-exchangeable hydrogen in kerogen from source rocks were measured from six Australian petroleum basins. Isotopic data for oils, oil sub-fractions and matching kerogens indicate that, in general, the individual components of an oil all have comparable δD values, with distinct isotopic clustering of oil families and source rocks from basins (Fig. 1). The weighted-average δD value of individual *n*-alkanes is usually identical to the saturate fraction and whole oil δD values. However a consistent trend of increasing δD with alkane chain length is observed in most oils derived from single sources, so that individual *n*-alkanes from one oil can vary in δD by 30‰ or more. This pattern likely reflects fractionations occurring during hydrocarbon cracking.

Hydrocarbon δD values (oils, oil fractions, and biomarkers) are in turn depleted in D by an average of 20‰ relative to the source kerogen (Fig. 2). A modest correlation between δD values for aromatic fractions of petroleum and formation waters indicates that about 50% of aromatic C-bound H has exchanged with water. Values of δD for whole oils and aliphatic and polar subfractions are uncorrelated with formation water δD values, indicating that essentially all C-bound H in these fractions has been conserved under reservoir conditions. On the other hand, δD values for acyclic isoprenoids and *n*-alkanes are essentially identical in all the petroleum systems examined, indicating that the large isotopic differences in these molecules due to primary biosynthetic effects have been erased. At the same time, variations in δD of 100‰ or more exist between *n*-alkanes from closely related oils of the Otway Basin, and apparently preserve the isotopic signature of a major climatic change. These apparently contradictory lines of evidence can be explained if (1) hydrogen exchange of C-bound H is extensive during petroleum generation, (2) the D/H composition of the bulk source rock – including water, organic H, and mineral H – is buffered against isotopic change, either as a result of its high organic and inorganic H content or by its low permeability, or both; and (3) the D/H ratios of petroleum hydrocarbons are essentially 'locked in' once an immiscible oil phase is generated and expelled from source rocks.

Figure 1: δD and $\delta^{13}\text{C}$ values of kerogens and oils from seven different basins, without distinguish among different source ages that may be represented within a basin. The data illustrate the power of combination of hydrogen and carbon stable isotopes to differentiate petroleum systems. Note that the y-axis is discontinuous. Dashed contour lines help visualizing isotopic ranges for each basin (Schimmelmann et al., 2004).

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Figure 2: δD and $\delta^{13}C$ values of kerogens and oils from four different basins, each with a distinct source rock age: Cooper Basin (Permian), Eromanga Basin (Middle Jurassic), Otway Basin (Early Cretaceous), and Gippsland Basin (Late Cretaceous/Early Tertiary). Small symbols indicate individual isotopic results, whereas large symbols represent basin-specific mean δ -values. For the Cooper, Eromanga, and Gippsland basins, dashed contour lines indicate the isotopic ranges of kerogens, and solid lines help visualize the isotopic ranges for oils. No ranges are marked for the Otway Basin, because δ -values of kerogens and oils are spread over large ranges and thus indicate heterogeneity of Otway Basin source rocks (Schimmelmann et al., 2004).

4.3. Hydrogen exchangeability and hydrogen isotopes in kerogen type-II from the New Albany Shale and the Exshaw Formation

Our PhD student Grzegorz Lis published a study in *Organic Geochemistry* (Lis et al., 2006) about irreversible but limited hydrogen isotopic exchange between kerogen from source rocks and formation water during thermal maturation. We compared the hydrogen isotopic composition and isotopic exchangeability of suites of Type-II kerogens from two basins, the New Albany Shale (Illinois Basin) and the Exshaw Fm. (Western Canada Sedimentary Basin). The largely marine-derived organic matter in these Late Devonian to Early Mississippian black shales had similar original stable isotope ratios, but today the suites of kerogens express gradients in thermal maturity that have altered their chemical and isotopic compositions. In both suites δD_n values increase with maturation up to a vitrinite reflectance of R_o 1.5 %, then level out. Increasing δD_n values suggest isotopic exchange of organic hydrogen with water-derived deuterium and/or preferential loss of 1H -enriched chemical moieties from kerogen during maturation. The resulting changes in δD_n values are altering the original hydrogen isotopic paleoenvironmental signal in kerogen, albeit in a systematic fashion (Fig. 3). The specific D/H response of each kerogen suite through maturation correlates with vitrinite reflectance R_o (here up to 1.5 %) and can therefore be corrected to yield paleoenvironmentally relevant information for a calibrated system. With increasing thermal maturity, the

abundance of hydrogen in kerogen that is isotopically exchangeable with water hydrogen (expressed as H_{ex} , in % of total hydrogen) first decreases to reach a minimum at $R_o \sim 0.8$ to 1.1 %, followed by a substantial increase at higher thermal maturity.

Figure 3: Relationships between the hydrogen stable isotope ratios of non-exchangeable hydrogen in kerogen (δD_n) and vitrinite reflectance R_o (a), and H/C elemental ratio (b) show distinct trends with increasing thermal maturity for the New Albany Shale and Exshaw Formation. δD_n values of kerogens from the New Albany Shale (Illinois Basin) and the Exshaw Formation (Western Canada Sedimentary Basin) indicate that the rate of D-enrichment with increasing maturity (maturity expressed as vitrinite reflectance R_o) is larger for the Exshaw Formation where the isotopic difference between organic and water hydrogen is also larger. Both paleoenvironments seem to have provided biomass with δD_n values around -160‰, which is a reasonable value for modern bulk biomass (Lis et al., 2006).

4.4. Invited Review: “Hydrogen isotopic (D/H) composition of organic matter during diagenesis and thermal maturation”

In 2004 the Editorial Committee of the journal *Annual Review of Earth and Planetary Sciences* had asked Schimmelmann to contribute an invited review article on the subject of hydrogen isotopes and organic matter maturation. Schimmelmann solicited expert help from collaborators Maria Mastalerz and Alex Sessions (a biogeochemist at Caltech). The review covered D/H in thermal maturation of organic matter in natural environments and in laboratory artificial maturation experiments. Figure 4 derives from this contribution and gives a comprehensive overview on organic matter maturation and D/H isotopic consequences (Schimmelmann et al., 2006).

Figure 4: Relationships between metamorphic zones, coal rank, diagenetic and maturity phases, hydrocarbon generation, and organic D/H changes (from [Schimmelmann et al., 2006](#)).

4.5. Novel equilibration method and applications for D/H measurements in kerogen

We published a paper in the journal *Rapid Communications in Mass Spectrometry* presenting a **novel hydrogen isotope equilibration method** for kerogen and other organic materials whereby exchangeable organic hydrogen in up to 49 organic samples in small silver cups is equilibrated with water hydrogen at 115°C overnight in a carousel ([Sauer et al., 2009](#)). The total organic hydrogen in equilibrated samples is subsequently converted to H₂ in a thermal conversion elemental analyzer (TC/EA) at 1420°C in the presence of excess glassy carbon. The resulting hydrogen pulses are carried in a stream of helium to a mass-spectrometer for on-line determination of D/H ratios. The new method is applicable to all non-volatile, solid organic compounds, e.g. kerogen, humic compounds, biological tissue, and synthetic polymers. The method was utilized to determine D/H ratios in kerogens from coals (see following section 4.6.) and from stratigraphic sequences across Permian/Triassic boundaries and thus aided in one additional paper in *Organic Geochemistry* ([Nabbefeld et al., 2010](#)) and one submitted manuscript (Nabbefeld et al., submitted to *Earth and Planetary Science Letters*).

4.6. Geochemical and isotopic consequences of a magmatic dike intrusion on coal

In 2007 we sampled a sequence of coals from a contact-metamorphic sequence where a magmatic dike had vertically intersected a coal seam in an underground mine in Illinois. Our isotope and other geochemical data from kerogens indicated surprising relationships between increasing thermal maturity, decreasing amounts of exchangeable hydrogen in kerogen and *decreasing* δD values of non-exchangeable hydrogen in kerogen. Most other environments with abundance of water express the opposite trend of *increasing* δD values with increasing thermal maturity. We attributed the coal's behavior near the dike to the fact that water and steam were limited when other hot gases were generated at the magmatic contact (e.g., hydrocarbon gases, nitrogen) and effectively dried the coal for the brief time period of contact metamorphism (Fig. 5). Our paper in the *International Journal of Coal Geology* described chemical, physical, and petrographic changes in these high-volatile bituminous coals ([Mastalerz et al., 2009b](#)). A second paper in *Geochimica et Cosmochimica Acta* described isotopic and other geochemical trends with increasing maturity ([Schimmelmann et al., 2009](#)).

Figure 5: A coal seam was vertically intersected by a magmatic dike (**upper panel**) resulting in rapid heating of coal and generation of steam and thermogenic gases. The highly permeable coal near the intrusion was effectively dried before it reached high enough temperatures for cracking reactions. Shale and paleosol/shale acted as poorly permeable barriers and limited hydrologic connectivity. (a) Increasing thermal maturity of coal is quantified by vitrinite reflectance R_o (%). (b) Decreasing amounts of exchangeable hydrogen (H_{ex}) in kerogen reflect the loss of chemical functional groups. (c) Decreasing δD_n values of non-exchangeable hydrogen in kerogen with increasing maturity contrast with other observations from water-rich environments and thus witness the absence of D-enriched water during heating ([Schimmelmann et al., 2009](#)).

4.7. Hydrogen stable isotopes and other geochemical tools in gas exploration

Hydrogen isotopic exchange with water hydrogen occurs when biogenic or thermogenic hydrocarbon gases are generated from sedimentary organic matter. In order to study compound-specific hydrogen and carbon stable isotope ratios of gas species in natural gas, we first developed a versatile analytical “GASIS” interface. Our article was published in *Rapid Communications in Mass Spectrometry* ([Henning et al., 2007](#)). The analytical GASIS method was then used to expand the utility of hydrogen stable isotopes in exploration for coalbed gases. Indiana’s coalbed gases in the southeastern Illinois Basin were characterized using diagnostic compound-specific hydrogen and carbon stable isotope ratios (among other geochemical and microbiological data). We published one initial paper in the journal *Organic Geochemistry* ([Strapoć et al., 2007](#)). Several related papers were subsequently published in the *International Journal of Coal Geology* ([Strapoć et al., 2008a](#)), in *Applied and Environmental Microbiology* ([Strapoć et al., 2008b](#)), and other journals. For example, we published two papers in 2009 and 2010 describing (a) **effects of coal storage** in air on physical and chemical properties of coal and on gas adsorption ([Mastalerz et al., 2009a](#)), and (b) consumption of trapped atmospheric oxygen and implications for measured gas quality using **coalbed gas** desorption in canisters ([Jin et al., 2010](#)). The latter publication also represents the major portion of Hui Jin’s M.Sc. thesis (Hui Jin subsequently joined the Ph.D. program at the Colorado School of Mines in summer 2009). Currently we have one additional gas-related paper submitted to the *AAPG Bulletin* (Strapoć et al., in review) and we have one invited review submitted about isotopes and other geochemical parameters in coalbed gases (Gao et al., in review).

PUBLICATIONS RESULTING FROM 2000-2010 DOE SUPPORT

Listings are in reverse chronological order;
bold numbers indicate peer-reviewed publications;
bold names identify personnel in our research group.

Seven of our graduate students benefitted from DOE support and served as authors and co-authors of presentations and publications:

Rachel Walker (Ph.D. 2005),
Grzegorz Lis (Ph.D. 2006),
Dariusz Strapoć (Ph.D. 2007),
Wilfrido Solano-Acosta (Ph.D. 2007),
Hui Jin (M.Sc. 2009),
Ling Gao (Ph.D. in progress),
Katarina Topalov (Ph.D. in progress).

a) PAPERS

1. **Gao**, Ling, Maria **Mastalerz**, and Arndt **Schimmelmann** (submitted, invited review) The origin of coalbed gas. [Chapter in a book to be published by the *North American Coalbed Methane Forum*; the book is planned to serve as a textbook for graduate students on coalbed methane technology that encompasses the complete scope of activities associated with coalbed methane production.]
2. Nabbefeld, Birgit, Kliti Grice, Arndt **Schimmelmann**, Peter E. Sauer, Michael E. Böttcher, and Richard Twitchett (submitted) Significance of $\delta D_{\text{kerogen}}$, $\delta^{13}C_{\text{kerogen}}$ and $\delta^{34}S_{\text{pyrite}}$ from several Permian/Triassic (P/Tr) sections. *Earth and Planetary Science Letters*.
3. **Strapoć**, Dariusz, Maria **Mastalerz**, Arndt **Schimmelmann**, and Agnieszka Drobniak (in press) Geochemical constraints on the origin and volume of gas of the New Albany Shale in the eastern part of the Illinois Basin. *AAPG Bulletin*.
4. Mao, Jingdong, Arndt **Schimmelmann**, Maria **Mastalerz**, P.G. Hatcher, and Y. Li (in press) Structural features of a bituminous coal and their changes during low-temperature oxidation and loss of volatiles investigated by advanced solid-state NMR spectroscopy. *Energy & Fuels*.
5. **Schimmelmann**, Arndt (invited review, in press) Carbon, nitrogen and oxygen stable isotope ratios in chitin. In: S. Neal Gupta, ed. *Chitin: Formation and Diagenesis*. Springer Geobiology Series.
6. **Schimmelmann**, Arndt, and Peter E. Sauer (invited review, in press) Methods to prepare water as H_2 for IRMS measurement of 2H . For: *Encyclopedia of Mass Spectrometry, Volume 5, Elemental and Isotope Ratio Mass Spectrometry* (Dwight Matthews, R. Sam Houk, Editors), Elsevier.
7. Mao, Jingdong, Xiaowen Fang, Yeqiang Lan, Arndt **Schimmelmann**, Maria **Mastalerz**, Ling Xu, and Klaus Schmidt-Rohr (2010) Chemical and nanometer-scale structure of kerogen and its change during thermal maturation investigated by advanced solid-state ^{13}C NMR spectroscopy. *Geochimica et Cosmochimica Acta* **74**, 2110-2127. <http://dx.doi.org/10.1016/j.gca.2009.12.029>
8. **Schimmelmann**, Arndt, and Grzegorz P. **Lis** (2010) Nitrogen isotopic exchange during maturation of organic matter. *Organic Geochemistry* **41** (1), 63–70. <http://dx.doi.org/10.1016/j.orggeochem.2009.01.005>
9. **Jin**, Hui, Arndt **Schimmelmann**, Maria **Mastalerz**, James Pope, Tim A. Moore (2010) Coalbed gas desorption in canisters: consumption of trapped atmospheric oxygen and implications for measured gas quality. *International Journal of Coal Geology* **81** (1), 64–72. <http://dx.doi.org/10.1016/j.coal.2009.10.010>
10. Nabbefeld, Birgit, Kliti Grice, Arndt **Schimmelmann**, Roger E. Summons, Ulrike Troitzsch, and Richard J. Twitchett (2010) A comparison of thermal maturity parameters between freely extracted hydrocarbons (Bitumen I) and a second extract (Bitumen II) from within the kerogen matrix of Permian and Triassic sedimentary rocks. *Organic Geochemistry* **41** (2), 78-87. <http://dx.doi.org/10.1016/j.orggeochem.2009.08.004>
11. **Schimmelmann**, Arndt, Andrea Albertino, Peter E. Sauer, Haiping Qi, Roland Molinie, and François Mesnard (2009) Nicotine, acetanilide and urea multi-level 2H -, ^{13}C - and ^{15}N -abundance reference materials for

- continuous-flow isotope ratio mass spectrometry. *Rapid Communications in Mass Spectrometry* **23**, 3513–3521. <http://dx.doi.org/10.1002/rcm.4277>
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