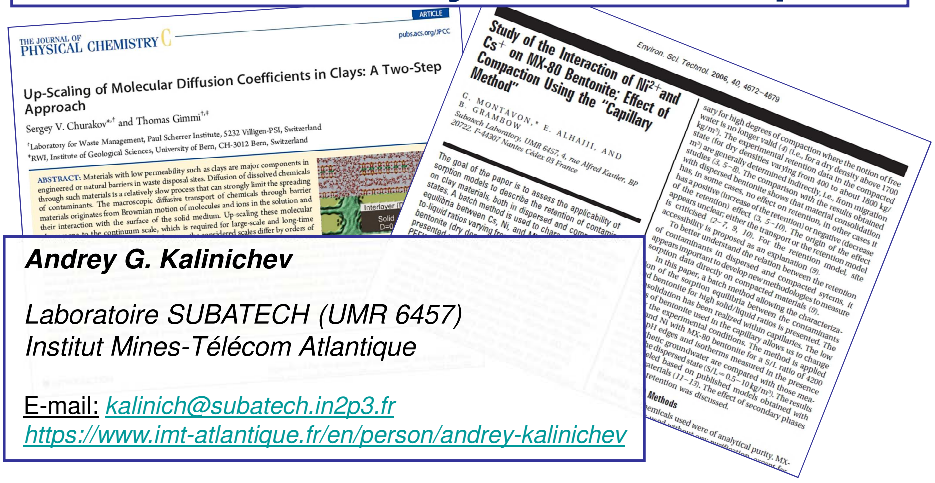
## NE-M1-PRI12ENP – Integrated Nuclear Engineering Project

# Molecular Modeling of Materials for Nuclear Waste Disposal Applications
# *Lecture 5* – The Anatomy of a Research Paper





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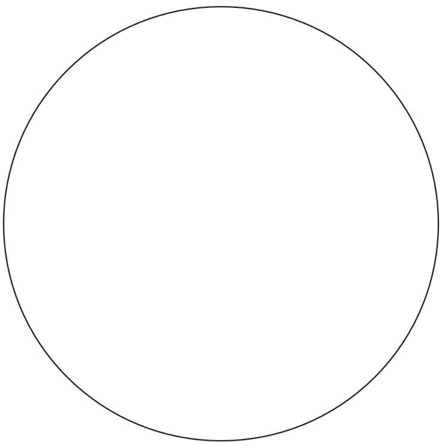
*https://www.imt-atlantique.fr/en/person/andrey-kalinichev*




## Progress of Knowledge (1)

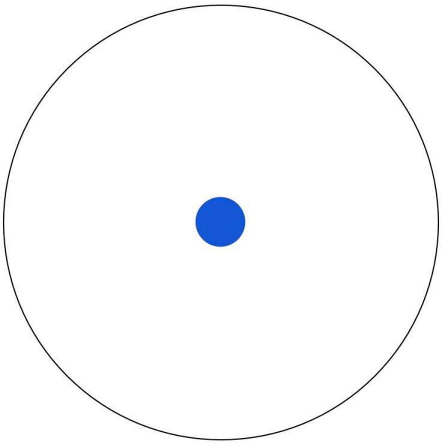
Imagine a circle that contains all of human knowledge:



Matt Might (http://www.businessinsider.com.au/the-illustrated-guide-to-a-phd-2012-3 )

## Progress of Knowledge (2)

By the time you finish elementary school, you know a little:



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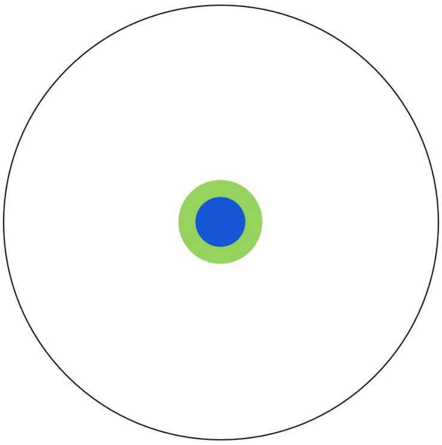
## Progress of Knowledge (3)

By the time you finish high school, you know a bit more:



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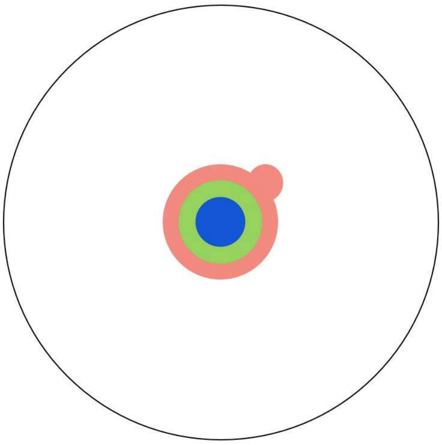
## Progress of Knowledge (4)

With an undergraduate degree, you gain a specialty:



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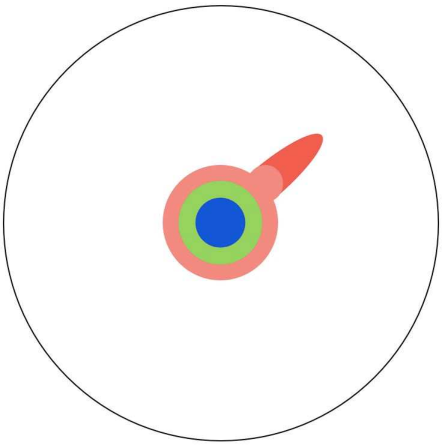
## Progress of Knowledge (5)

A master's degree deepens that specialty:



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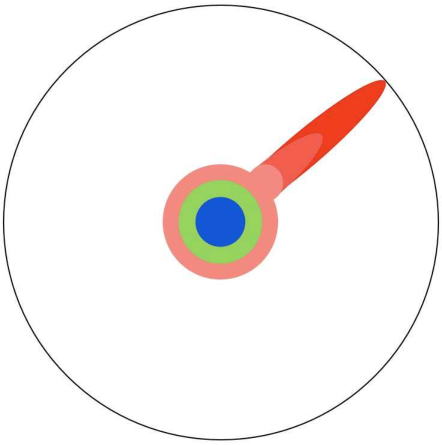
## Progress of Knowledge (6)

Reading research papers takes you to the edge of human knowledge:



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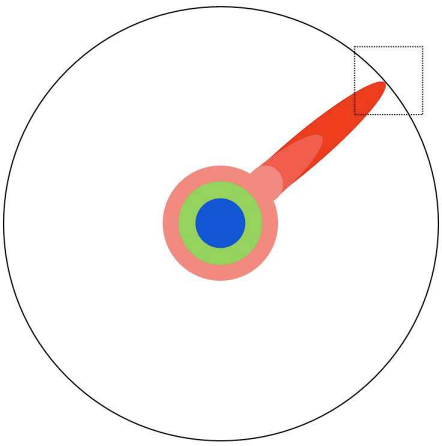
## Progress of Knowledge (7)

Once you're at the boundary, you may want to focus on a single research topic (your possible future PhD project):



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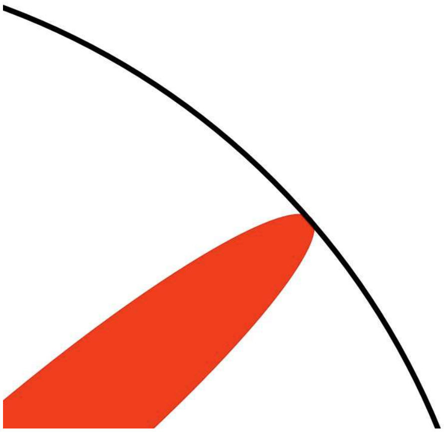
## Progress of Knowledge (8)

You will push at the boundary for a few years:



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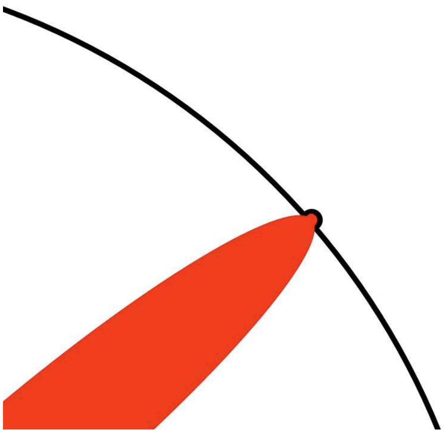
## Progress of Knowledge (9)

Gradually, the boundary may give way:



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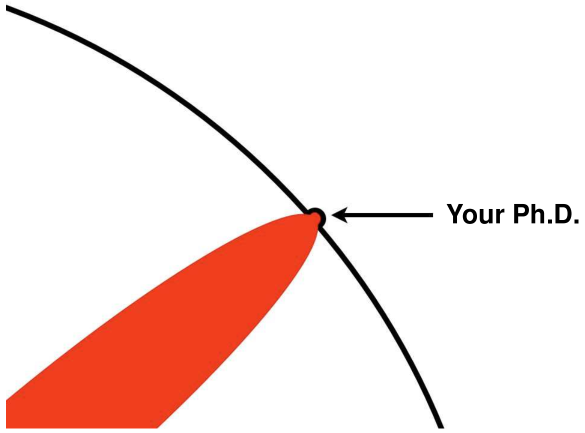
## Progress of Knowledge (10)

And, that dent you've made is called a Ph.D.:

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## Progress of Knowledge (11)

Of course, the world will look different to you now:

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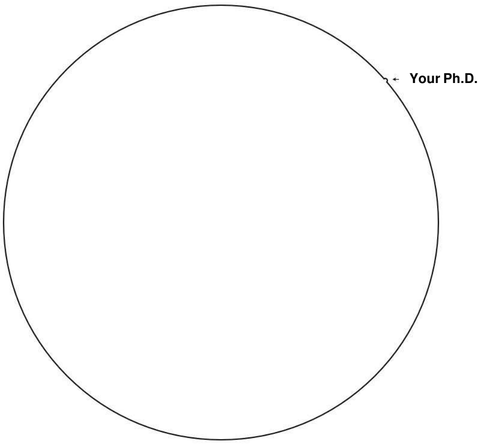
## Progress of Knowledge (12)

But never forget the bigger picture:

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## Read First!

***"Just a couple of months of hard work in the lab can save you the whole two hours spent in the library"***
(source unknown)

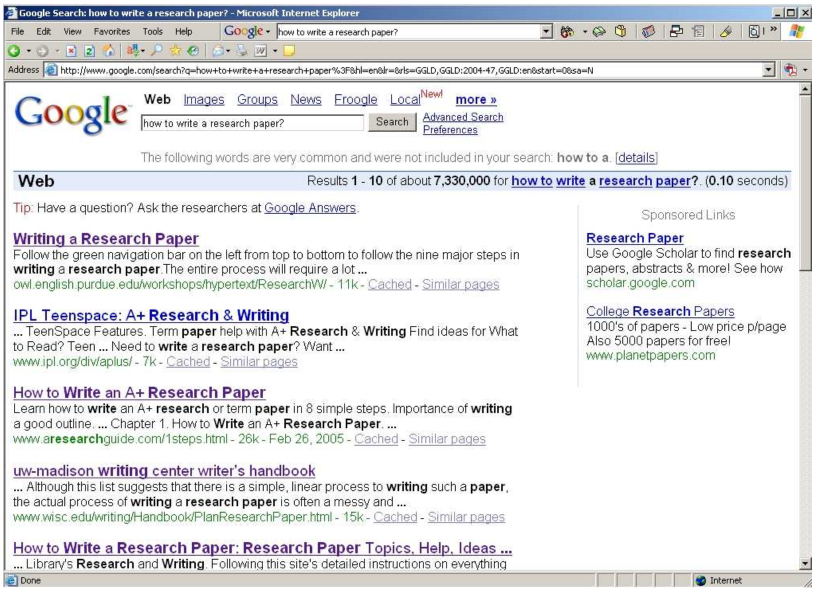
- Research is more **reading**, than **writing** 10 : 1, possibly 100 : 1
- **Read** before starting your research project
- **Read** during your research project
- **Read** while writing your paper
- **Organize** your reading notes, lists of literature references, photocopies, reprints, etc.
- One does not even need to go to a library anymore: **on-line databases and archives** of research journals are available
- Know and regularly read your **professional research journals**
- Get to know **who is doing what** in your chosen research area (not necessarily from your Department or University, or even from your country)
- Don't be shy contacting people and asking for reprints or advice

## While Reading Research Papers, Think About These Important Questions

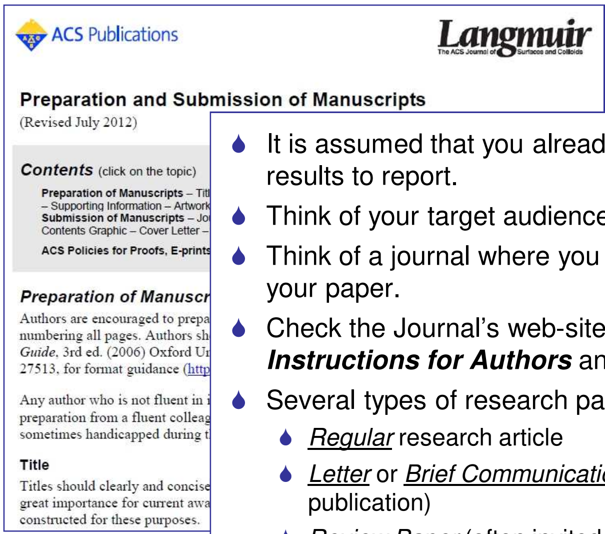
- Why this particular research was performed?
- What methods of measurements and/or calculations were used and why?
- Are there any default / implicit assumptions or approximations used in the measurements / calculations / interpretation of the results?
- Are there any limitations to the experimental / theoretical approaches used?
- Are the results statistically meaningful?
- What are the sources of errors and inaccuracies associated with the methods of measurements or calculations used by the authors?
- Formulate your own opinion of the paper: 2-3 strong points of the given paper and 2-3 weak points of the paper.



## Collect Information



## Writing a Research Paper


ACS Publications

Langmuir

The ACS Journal of Surfaces and Colloids

Preparation and Submission of Manuscripts

(Revised July 2012)

*Contents* (click on the topic)

**Preparation of Manuscripts** – Titl
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**Submission of Manuscripts** – Jo
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**ACS Policies for Proofs, E-prints**

*Preparation of Manuscr*

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**Title**

Titles should clearly and concise
great importance for current awa
constructed for these purposes.

- It is assumed that you already have some research results to report.
- Think of your target audience. Who are your readers?
- Think of a journal where you are planning to submit your paper.
- Check the Journal's web-site or recent issues for ***Instructions for Authors*** and ***Guide for Submission***
- Several types of research papers:
  - *Regular* research article
  - *Letter* or *Brief Communication* (limited size, but faster publication)
  - *Review Paper* (often invited by the Journal's Editor)

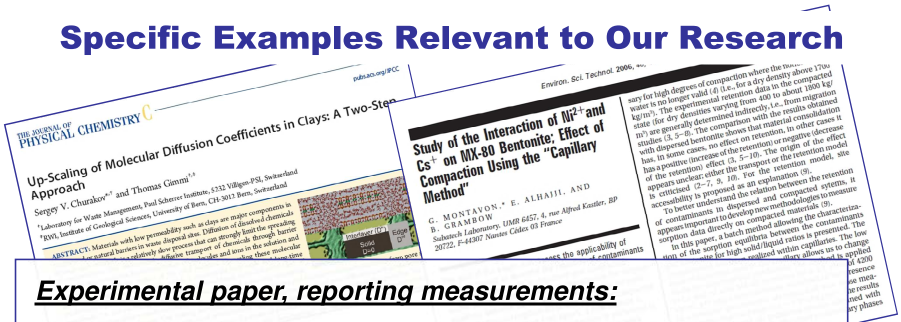


## General Form of a Research Paper

- The **objective** of organizing a research paper is to allow people to read your work **selectively and quickly**:
  - some may be interested in just the methods;
  - or in a specific result, the interpretation;
  - or perhaps just want to see a summary to determine if it is relevant to their own study.
- Most journals require the submitted manuscripts to be divided into sections, following a general standard (some variations are possible):
  - **Title page**
  - **Abstract**
  - **Introduction**
  - **Methods and Materials**
  - **Results**
  - **Discussion**
  - **Summary or Conclusions**
  - **Literature References**
  - **Tables, Figures, and Captures to them**

May be further divided into sub-sections

# Specific Examples Relevant to Our Research




***Experimental paper, reporting measurements:***

Montavon, G., Alhajji, E., and Grambow, B. (2006) Study of the interaction of $Ni^{2+}$ and $Cs^{+}$ on MX-80 bentonite; Effect of compaction using the "capillary method".

*Environmental Science & Technology,* **40,** 4672-4679.

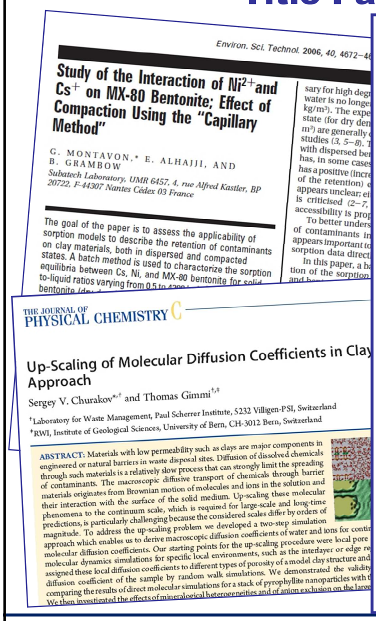
***Theoretical modeling paper, reporting results of simulations:***

Churakov, S. V. and Gimmi, T. (2011) Up-scaling of molecular diffusion coefficients in clays: A two-step approach.

*Journal of Physical Chemistry C*, **115,** 6703–6714.



# Title Page and Abstract




- **Title** should be **concise** and **informative**
- Include the names and addresses of all authors
- **Abstract** - a single paragraph (200-300 words) summary of your work. In a minute or less a reader should be able to learn:
  - the rationale behind the study
  - general approach to the problem
  - pertinent results
  - important conclusions or new questions.
- **One or two sentences each** for:
  - purpose of the study - hypothesis, overall question, objective
  - brief description of the experiment or the modeling approach
  - results, including *specific quantitative data*;
  - results of any statistical analysis
  - important conclusions or unresolved questions that follow from the work
- Abstract is typically written **after** the manuscript is complete

## Introduction

- The purpose of an introduction is to explain to the reader the rationale behind the work. Typically – 2-3 pages of the manuscript.
- Authors should be able to defend their work based on the information provided in the Introduction.
- It places the work in a general scientific context, and enables the reader to understand and appreciate its objectives.
- General context ⇒ context of a specific discipline ⇒ specific problem.

**INTRODUCTION**

Compacted smectite clays, such as bentonites, possess near zero hydraulic conductivity,[1] which makes molecular diffusion the dominant transport process for aqueous species. The diffusive mass transport of cationic species is further retarded by sorption on the surfaces of negatively charged clay particles. Due to such exceptional transport properties, clay-rich rocks are considered as a buffer and backfill material for high-level radioactive waste repositories worldwide.[2−5] Clays are also used as sealing materials in landfill sites to prevent the spreading of toxic substances into the surroundings.[6−8]

To predict diffusive migration of ions and water in a porous medium with porosity $\varepsilon$ on a macroscopic scale, continuum models are used[9]

$$\varepsilon\frac{\partial C_i}{\partial t} = -\nabla\cdot J_i + R_i = \nabla\cdot(\varepsilon D_p^{REV}\nabla C_i) + R_i \quad (1)$$

In these models, solutes are transported according to the diffusive flux $J_i = -\varepsilon D_p^{REV}\nabla C_i$ and retarded or released by means of chemical reactions $R_i$ due to precipitation/dissolution of solid phases and sorption/desorption on the surfaces of minerals. Such a separate description of diffusion and sorption (and/or pre-

depends on the composition of the system. In typical applications, eq 1 is solved numerically on a grid. The smallest possible volume element of the grid is given by the representative elementary volume (REV). At the REV scale the porous medium is replaced by a conceptual macroscopic medium by means of some averaging over microscopic heterogeneities. The pore diffusion coefficient, $D_p^{REV}$, thus, represents average properties of the medium at the REV scale.[10]

Diffusion of ions and water in porous media is restricted to the porous space occupied by solvent, and thus the average macroscopic diffusion coefficient in porous media depends on the specific pore space topology in the sample and the strength of fluid−surface interaction. Numerous attempts have been undertaken to relate diffusion coefficients in porous media to those of the same solute in bulk solution $D_0$. The bulk diffusion coefficients are typically reduced with a so-called formation factor $F$[11]

$$D_p^{REV} = \frac{1}{F} D_0 \quad (2)$$

For a "simple" porous medium with large pores, it has been suggested that the formation factor can be approximated by two geometric factors, one accounting for an increased length of the diffusion path (tortuosity $\tau^2$) and the other accounting for the

**Introduction**

Bentonite is a clay-based natural material which may serve as an engineered barrier in deep geological repositories for radioactive waste (e.g., ref *1*). The transport of contaminants in water-saturated porous clay systems is controlled by sorption (e.g., refs *2, 3*). This interaction is typically modeled based on sorption data obtained from batch sorption measurements performed with dispersed bentonite, i.e., on systems with low solid-to-liquid (S/L) ratios. The literature on sorption of contaminants on dispersed bentonite is voluminous (e.g., refs *2, 3*).

It is necessary to ensure that sorption parameters obtained on dispersed materials are able to describe the sorption processes in compacted media. This appears notably necessary for high degrees of compaction where the notion of free water is no longer valid (*4*) (i.e., for a dry density above 1700 kg/m³). The experimental retention data in the compacted state (for dry densities varying from 400 to about 1800 kg/m³) are generally determined indirectly, i.e., from migration studies (*3, 5−8*). The comparison with the results obtained



## Introduction

- Provide a broad scientific context. Describe the importance / significance of the study. Why was this worth doing in the first place? **"So what?"**-question.
- Defend the model / system / method - why study this approach or system? What are the advantages? You might comment on its suitability from a fundamental scientific point of view or indicate practical reasons for using it.
- Provide a rationale. State your specific hypotheses or objectives, and describe the reasoning that led you to select them.
- Very briefly describe the experimental design or the modeling approach and how they will accomplish the stated objectives.
- Organize your ideas, making one major point with each paragraph. If you make the four points listed above, you will need a minimum of four paragraphs.
- Be as precise and specific as possible - do not oversimplify.
- Think of your potential readers and remember that they are not necessarily as familiar with the subject as you are.
- Present background information only as needed in order to support a position. The reader does not want to read everything you know about a subject.

# Methods and Materials

- ***Keep this section*** as ***concise*** as you possibly can. People will want to read this selectively (often printed in small print). The reader may only be interested in one formula or part of a procedure.
- On the other hand, ***give enough detailed information***, so that a knowledgeable reader should be able to determine whether or not your methods were appropriate and to reproduce your results. A scheme of experimental setup is appropriate here.
- This should be the easiest section to write. A ***typical lab notebook should contain all of the information*** that one needs for this section.
- ***Report the methodology***, not details of each procedure that employed the same methodology. This section is not a set of instructions.
- ***Generalize*** - report how procedures were done, not how they were specifically performed on a particular day. Always think about what would be relevant to an investigator at another institution, working on their own similar project.
- If well documented procedures were used, report the procedure by name, perhaps with a literature reference.
- Omit all explanatory information and background - save it for the discussion.
- Omit information that is irrelevant to a third party, such as what color ice bucket you used, or which individual logged in the data.



# Methods and Materials

- For a theoretical / computational paper all the theoretical derivations and equations / methods used in the study should be introduced and described here.
- For an experimental paper reporting the results of measurements a scheme of experimental setup is appropriate in this section.

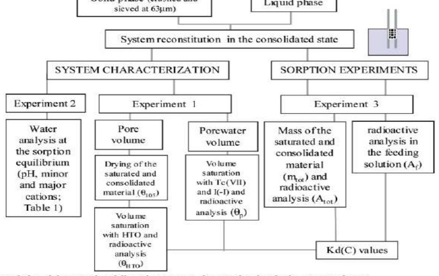



**FIGURE 1. Description of the procedure followed to measure the retention data in the compacted state.**

## METHOD

**MD Simulation.** Molecular dynamics simulations were performed using the LAMMPS package[39] developed at Sandia National Laboratory. The interaction between atoms and molecules was taken into account using the CLAYFF force field.[40] The corresponding flexible SPC water model[40] has been used throughout the simulations. The simulations were performed in *NVT* ensemble with a time step of 1 fs. A Nose−Hoover chain of thermostats[41,42] with the temperature dumping parameter equal to 1 ps was applied to keep average temperature at 300 K during the simulations. The parameters of the simulation box for *NVT* simulations were obtained from a set of *NPT* simulations at the pressure of 1 bar. The systems studied were equilibrated for 500 ps followed by a 110 ns long trajectory which was used for the analysis of the distribution of water molecules and their diffusivities. Diffusion coefficients of the water molecules along the direction of Cartesian coordinates were derived from the mean square displacement of the molecules using the Einstein relationship,[43] as indicated in eq 5.

**RW Simulations.** Random walk simulations in a heterogeneous domain were performed using the predictor-corrector scheme suggested by LaBolle et al.[44] to account correctly for heterogeneous local diffusion coefficients

$$\delta x = Z\sqrt{2D(x(t))\Delta t} \qquad (7)$$

$$x_k(t + \Delta t) = x_k(t) + Z\sqrt{2D(x_k(t) + \delta x)\Delta t} \qquad (8)$$

In this algorithm, the random number Z is drawn to generate a predictor step $\delta x$ according to eq 7. Then the particle is moved using the same random number Z but the diffusion coefficient $D(x_k(t) + \delta x)$ obtained at the position $x(t) + \delta x$ (eq 8). We used the Gaussian distribution to obtain Z, but other distributions can also be used. The appropriateness of this algorithm has been verified by La Bolle et al.[44,45] and by ourselves through comparisons with analytical solutions for simple heterogeneous arrangements. A zero diffusion coefficient was attributed to impermeable regions, such that the system of eqs 7 and 8 also

# Methods, Materials, and Models

**Materials and Methods**

**Materials.** All chemicals used were of analytical purity. MX-80 bentonite was used without any purification, except for some sorption tests realized with Ni in the dispersed state, where bentonite was treated with $H_2O_2$ (S/L = 10 kg/m$^3$; NaCl 0.05M; $H_2O_2$ 12%, $T$ = 70 °C; five treatments) to selectively remove organic matter (*14*). The montmorillonite fraction amounts to 84% (*11*). Natural Ni and Cs were found in MX-80 bentonite with amounts of 5.4 mg/kg and 0.11 mg/kg, respectively (*15*). Experiments performed under acidic conditions (pH 2.5, $NaNO_3$ 0.05M) showed that about 65% of the inventories of Cs and Ni were mobilizable (*15*). A water content of 8% was determined by drying at 105 °C for 12 h and taken into account for the calculation of the bentonite concentration in the dispersed state. HTO, $^{63}$Ni, and $^{137}$Cs (with carrier) were obtained from CERCA−FRAMATOME, AMERSHAM, and CEA/DAMRI, respectively. Capillaries in PEEK of 1 mm internal diameter were used for the experiments realized with compacted bentonite.

**Sorption Study.** All experiments were performed at $T = 23 \pm 3$ °C. Sorption data were measured using a typical water composition of the claystone of the Bure site (see Table 1). Two types of data sets were collected: in the first case, sorption is studied at initial fixed metal ion concentration as a function of pH (sorption pH edges) and in the second case, sorption was measured as a function of metal ion concentration at constant pH (sorption isotherms). For the measurement of pH edges, the pH value was varied between 4 and 9 using NaOH and $HClO_4$ stock solutions. For fixing the pH above a value of 4 for sorption studies, MES (2-(N−morpholino)ethane-sulfonic acid), MOPS (3-(N−morpholino)propane-sulfonic acid), and/or TRIS (tris(hydroxymethyl)-aminomethane) buffers at a concentration of $2 \times 10^{-3}$M were used. They are known to not alter the sorption behavior of metal ions on clay materials in the dispersed state (*12*). Some

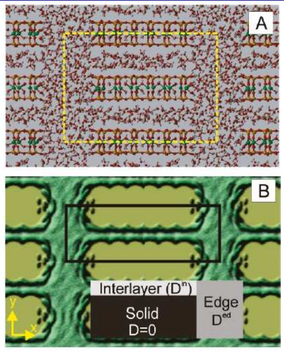



**Figure 1.** (A) Snapshot from MD simulations of pyrophyllite particles separated by two water layers. Oxygen, hydrogen, silica, and aluminum atoms are shown as red, gray, yellow, and green spheres, respectively. The simulation supercell is shown by the yellow dashed line. (B) A surface plot of the 2D probability density profile of water molecules from molecular dynamics simulations. Peak areas correspond to long residence times. In the overlay, light gray and gray areas indicate interlayer space and interparticle porosity, respectively, as assigned for the RW simulations. The diffusion coefficients $D^{in}$ and $D^{ed}$ for these pore spaces were obtained from short (200 ps) MD trajectories resident in the corresponding domains. The solid phase domain impenetrable for water is shown as a black area. The simulation cell for the RW simulations is shown by the solid black line.



# Results

- The purpose of this section is to **present and illustrate your findings**.
- Use **figures and tables** to present results most effectively.
- This should be a completely objective report of the **results.**
- **Save all interpretation for the discussion.**
- **Point the reader** to observations that are **most relevant**.

**Table 4. Input Parameters and Results of the Different Simulations for the Heterogeneous Clay Structure**[a]

| run | particle number | $D_l^{\Omega}(x)$ [ $10^{-9}$ m$^2$ s$^{-1}$] | $D_x$ [ $10^{-10}$ m$^2$ s$^{-1}$] | $D_y$ [ $10^{-10}$ m$^2$ s$^{-1}$] | $D_x/D_y$ | $F_x$ | $F_y$ | $G_x$ | $G_y$ |
|---|---|---|---|---|---|---|---|---|---|
| homog. local *D* | 2 k | 2.3 | 9.2 ± 0.0026 | 4.9 ± 0.0013 | 1.88 | | | | |
| homog. local *D* | 2 k | 2.3 | 8.8 ± 0.0029 | 4.9 ± 0.0015 | 1.78 | | | | |
| homog. local *D* | 10 k | 2.3 | 8.7 ± 0.0015 | 4.7 ± 0.00082 | 1.85 | 2.63 | 4.86 | 2.63 | 4.86 |
| homog. local *D* | 10 k | 2.3 | 9.0 ± 0.0010 | 4.8 ± 0.00084 | 1.88 | 2.57 | 4.82 | 2.57 | 4.82 |
| homog. local *D* | 10 k[b] | 2.3 | 8.8 ± 0.013 | 4.8 ± 0.0071 | 1.86 ± 0.021 | 2.60 | 4.84 | 2.60 | 4.84 |
| heterog. local *D* pyrophyllite | 10 k | $2.92D_{il}^{\Omega}$ $1.98D_{ed}^{\Omega}$ | 9.2 ± 0.0008 | 5.0 ± 0.00050 | 1.84 | 2.50 | 4.60 | 2.99 | 5.51 |
| heterog. local *D* montmorillonite | 10 k | $1.20D_{il}^{\Omega}$ $1.90D_{ed}^{\Omega}$ | 5.4 ± 0.0006 | 3.2 ± 0.00018 | 1.69 | 4.26 | 7.19 | 2.48 | 4.18 |
| heterog. mineralogy, 30% illite | 10 k | 2.3 | 8.67 ± 0.0007 | 4.95 ± 0.00051 | 1.76 | 2.66 | 4.69 | 2.66 | 4.69 |
| heterog. mineralogy, 70% illite | 10 k | 2.3 | 7.61 ± 0.0009 | 5.31 ± 0.00054 | 1.45 | 3.01 | 4.35 | 3.01 | 4.35 |
| heterog. mineralogy, 100% illite | 10 k | 2.3 | 8.85 ± 0.0007 | 6.19 ± 0.00044 | 1.40 | 2.61 | 3.66 | 2.61 | 3.66 |
| heterog. mineralogy, 100% illite | 10 k | 2.3 | 8.67 ± 0.0006 | 6.02 ± 0.00029 | 1.42 | 2.67 | 3.80 | 2.67 | 3.80 |
| anions | 10 k | 1.9 | 4.09 ± 0.0003 | 2.63 ± 0.00038 | 1.55 | 5.62 | 8.74 | 4.63 | 7.17 |

[a] $D_x$, $D_y$: Sample-scale diffusion coefficients parallel ($x$) and perpendicular ($y$) to bedding; $F_x$, $F_y$: Formation factors in $x$ and $y$ direction; $G_x$, $G_y$: Geometric tortuosities in $x$ and $y$ direction;. [b] Means and errors estimated from the two runs with 10 k particles.

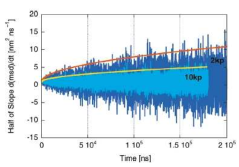



**Figure 7.** Variability of half of the local slope of the mean square displacement ($x$ direction) with respect to time. The mean value corresponds to the average diffusion coefficient of the medium. The dark blue curve was obtained for 2000 walker particles and the light blue curve for 10 000 walker particles. The orange and the yellow curve illustrate the time dependence of the fluctuation amplitude according to eq 13.

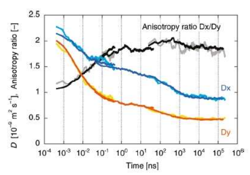
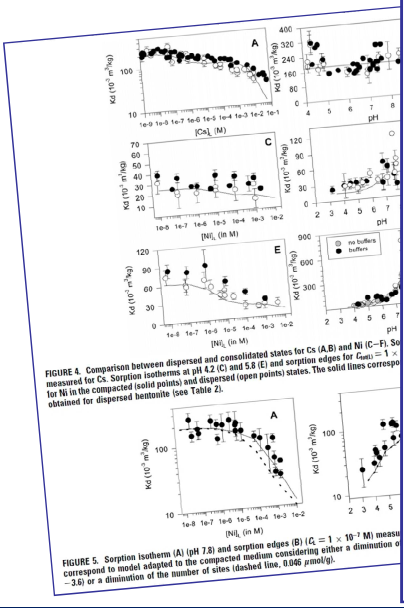



**Figure 8.** Development of average diffusion coeffcients in horizontal ($D_x$) and vertical ($D_y$) directions and of anisotropy ratio with simulation time. The data were calculated from five simulations with different initial particle distributions and over different simulation times, using either 2000 particles (bright lines) or 10 000 particles (dark lines).

simulations, the "effective" particle density available for the mean

## Results



- **Analyze your data**, then prepare the analyzed (converted) data in the form of a figure (graph), table, or in text form.
- Do not present the same data more than once (**either in a figure or in a table**).
- Present the results in order of their **importance and relevance to further discussion**, not in a sequence in which they were obtained.
- **Distinguish** material that should normally be included in a research article from any raw data or other appendix material that would not be published. (Such material should not be submitted at all unless requested by the Editor or a Reviewer of the manuscript).
- Typically figures and tables are included in the back of the manuscript (following Literature References).
- Each figure and table must be sufficiently complete that it could stand on its own, separate from text. **Formulate descriptive figure and table captions**.
- Typically 3-5 pages.



## Discussion

- The objective is to provide an **interpretation of your results** and support for all of your conclusions, using evidence from your experiment and generally accepted knowledge, if appropriate.
- **Explain all of your observations** as much as possible, focusing on mechanisms.
- Use **figures and tables** to present your observations most effectively.
- Interpret your data in the **discussion in appropriate depth**:
  - When you explain a phenomenon you must explain mechanisms.
  - If your results differ from your expectations or someone else's results for similar systems, explain why that may have happened.
  - If your results agree, then describe the theory that the evidence supported.
  - It is never appropriate to simply state that the data agreed (or disagreed) with expectations, and let it drop at that.
- **Decide** if each hypothesis is supported, rejected, or if you cannot make a confident decision. Do not simply dismiss a study or part of a study as "inconclusive."
- **Make suggestions** how the experiments/calculations might be **modified**, if necessary, in order to properly test the hypotheses or accomplish the objectives.
- Try to offer **alternative explanations** if reasonable alternatives exist.

# Summary or Conclusions

- Always keep the **big picture** in mind, where do you go next?
- One paper will not answer all questions, best studies open up new directions of research.
- What questions remain?
- Be creative, and don't be afraid to speculate based on your results and their interpretations.

■ SUMMARY AND CONCLUSIONS

We presented a two-step simulation approach which enables us to derive the average diffusion coefficient of water and ions in complex, heterogeneous porous media based on the results of molecular simulations performed in this study and reported in

We found that the clay structure map which we used in the present simulations leads to values in a range comparable to those measured but does not match exactly some transport properties of real media. The geometry factors G calculated for a montmorillonite structural map are similar to experimental values for illites or kaolinites and to experimental values for bentonites at somewhat smaller bulk densities but somewhat lower than experimental values for montmorillonites at the same densities. These discrepancies can be explained by the imperfectness and the simplicity of the clay structure map used in the simulations. Some generally unknown details of the pore-scale structure such as the closeness of the contacts between different particles are important for the overall results. The sample map used in the simulations, $200 \times 150$ nm$^2$, is small. For this size, larger circularities of the particles than for real samples had to be used, and the characteristic distribution functions (notably the particle sizes) had to remain relatively narrow. Real samples are likely to have larger structural heterogeneities and broader distributions of particle sizes and shapes, which will lead to larger tortuosities. These discrepancies will be addressed in the future by using a representative set of structure maps tailored to a specific sample.

So far we have considered the mobility of water in porous media or of aqueous ions at chemical equilibrium. To describe the relaxation of a nonequilibrium system toward the equilibrium state the immobilization of ions due to strong site-specific sorption and/or incorporation into the solid phase need to be considered at the continuum scale through the source/sink term in eq 1, which accounts for the equilibrium ion distribution between aqueous (mobile) and sorbed (immobile) states. Technically speaking, site-specific ion sorption on the surface of minerals can also be included in the pore-scale random walk simulation.[63] The practical efficiency of both approaches will depend on the system-specific questions to be answered. Considering general-purpose simulation of multispecies transport with chemical reactions the coarse-grain description of the system that combines molecular simulations according to eq 5, pore scale modeling according to eq 6, and continuum transport simulations will be most robust.

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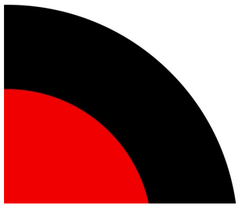



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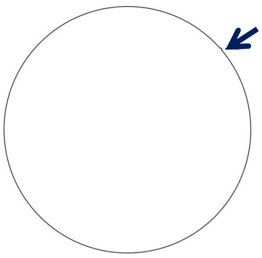

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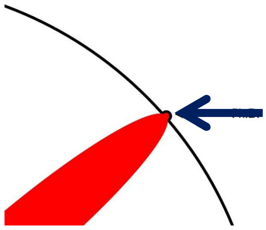

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## Literature References

■ ACKNOWLEDGMENT

The simulations were performed in the Swiss Centre of Scientific Computing (CSCS-Manno). The authors acknowledge the partial financial support of the project by Nagra.

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- **Acknowledge** the sources of financial support for you work.
- **Acknowledge** essential technical assistance and discussions with persons who are not co-authors of the manuscript.
- When you refer to information, distinguish data generated by your own studies from published information.
- List all literature cited in your manuscript.
- Different journals have different formats for references.
- In a proper research paper, only primary literature is used (original research articles authored by the original investigators).
- A web site is generally not an appropriate reference.
- If you are citing an on-line journal, use the journal citation (name, volume, year, page numbers).
- Typically, a regular research paper has 20 to 50 literature references.

## Presenting Research at a Conference – The Anatomy of a Conference Talk (I)

- Typically, **only 15-20 minutes** to present your results
  ⇒ ~10-15 slides at most
- **Every word counts**, every slide or figure counts
- There in **no way to give an extensive research background** and all the supporting information for your project in such a talk
- **Graphics** is much more preferable to tabulated data or wordy descriptions
- **Font size** of the figures should be **larger**, than one typically uses in  printed manuscript
- **Always keep your audience in mind** the same way you keep your readers in mind while writing a research paper



## Presenting Research at a Conference – The Anatomy of a Conference Talk (II)

Structure of a talk may be similar to that of a paper, but
**it might be beneficial to use it backwards**:

- Put your work into the context of general scientific area and formulate the problem you are going to address by 2-3 slides
- Focus only on 2 or 3 specific results and/or conclusions
- Clearly and concisely state your conclusions
- Support these statements by data
- Use only the most essential data, skip the details
- "Methods" can be skipped completely or mentioned just briefly

## Questions for the final paper / report on one of the 21 topics, e.g., 1 – clays; 2 – cement; 3 – $TiO_2$ surfaces; 4 – corrosion; 5 – organics, etc. (https://moodle.imt-atlantique.fr/course/view.php?id=407 ) (Please use only as a guidance)

- What molecular modeling method was used and why?
- Was it a fully atomistic simulations, or some simplified models were used?
- What other approximations were used in the modeling?
- What was the number of particles in the simulations? Was it big enough for the specific problem? Was it small enough to make the simulations computationally efficient?
- How long-range electrostatic interactions were handled in the simulations? Was it important for the given problem?
- What kind of boundary conditions were applied to the simulation box? Why?
- What properties of the system were calculated from the molecular simulation?
- Make a qualitative assessment of the accuracy for the calculated properties given the number of atoms in the simulated system and the duration of the simulation.
- What other properties would you additionally calculate from the same simulations for the same system?
- Formulate 2 or 3 strong points of the given molecular simulation paper and 2 or 3 weak points of the paper.