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Numerical Modelling of Sediment Generation

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Dissertation presented in partial fulfillment of the requirements for the degree of Doctor of Science (PhD): Geology

April 2020

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Preface

This PhD gave me the opportunity to venture into the exciting world of programming and establish a strong foothold in Python. Combined with my geology knowledge it served this topic well.

Instructies van de faculteit:

In het voorwoord wordt de algemene doelstelling van het werk samengevat in enkele regels en worden personen, diensten of firma's bedankt voor hun medewerking bij het tot stand komen van het werk.

De naam van firma's en personen uit deze firma's mogen slechts worden vermeld mits hun uitdrukkelijke toelating én na overleg met de supervisor(en)! Steeds wordt de supervisor(en) vermeld, de verantwoordelijke en eventueel de personen die rechtstreeks geholpen hebben bv. door het ter beschikking stelling van meetresultaten, faciliteiten. Ook de instantie die eventueel een doctoraatsbeurs heeft toegekend wordt bedankt (bv. FWO, IWT, . . .).

Abstract

Sediment generation is one the major challenges still remaining in sedimentary petrology.

Instructies van de faculteit:

In een beknopte tekst van maximum 2 pagina's worden de belangrijkste doelstellingen en besluiten geformuleerd, zowel in het Nederlands als in het Engels. Zulke samenvattingen kunnen worden gebruikt in wetenschappelijke verslagen van het departement of de faculteit. Het Engels moet vlekkeloos zijn.

Beknopte samenvatting

...

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In een beknopte tekst van maximum 2 pagina’s worden de belangrijkste doelstellingen en besluiten geformuleerd, zowel in het Nederlands als in het Engels. Zulke samenvattingen kunnen worden gebruikt in wetenschappelijke verslagen van het departement of de faculteit. Het Engels moet vlekkeloos zijn.

Contents

List of Figures

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Instructies van de faculteit:

De hoofdstukken: Elk hoofdstuk is ingelast met een bepaald doel voor ogen. Dit doel wordt vermeld in de eerste paragraaf van elk hoofdstuk. Naargelang de aard van de tekst (experiment, uitvoering, theoretische ontwikkeling, ...) volgen de paragrafen elkaar op. Beweringen worden altijd gestaafd, hetzij door eigen experimenten, hetzij door een theoretische afleiding, hetzij door verwijzingen naar de literatuur. Elk hoofdstuk eindigt met een kort samenvattend besluit waarbij nagegaan wordt in hoeverre de doelstelling van het betrokken hoofdstuk verwezenlijkt is. De deelbesluiten moeten de lezer automatisch leiden naar het algemeen besluit aan het einde van het werk.

CHAPTER **1**

Introduction

Instructies van de faculteit:

De inleiding situeert de problematiek, beschrijft de stand van de huidige kennis terzake, omschrijft de voornaamste doelstelligen van het werk, samen met de beperkende randvoorwaarden en de ter beschikking gestelde middelen en poneert de belangrijkste stellingen.

1.1 General introduction

Sediment generation

1.2 Parent rock characterization

A general approach to the characterization of parent rocks should be established if one wants to be the input of a sediment generation model to be applicable to multiple input conditions. Therefore, the descriptor as proposed by Griffiths 1952, 1961 was extended to apply to parent rocks. The Generalized Griffiths Descriptor (GGD). *A*

1.3 Model architecture

1.3.1 Main

The main code block runs the entire model. It can access all the global parameters and functions. When the model is run, input data will be requested to be provided. This can be done by pointing to a path or opening the file via the GUI. Next these data will be pre-processed to be in a format suitable for further analysis. The mechanical weathering module is then run, which will retrieve data from the input module as well as from the mineral properties and boundary conditions modules. As soon as grains and rock fragments become available, the chemical weathering module starts and with it the precipitation module. The mass balance module is already taken everything into account and bookkeeping all grains and rock fragments over different grains size classes and mineralogical classes. The user may specify at which time steps an output of the data is requested. The output data can then be post-processed to be presented as graphs and figures.

1.3.2 Input & pre-processing

Necessary user input data consists of three parts: modal mineralogy, relative interface frequencies and crystal size distribution. (i) The modal mineralogy contains the volume proportions of the minerals present in the source rock. See chapter 4. (ii) The relative interface frequencies contain the fractions of all present mineral interface occurrences. See chapter 5. (iii) The crystal size distribution (CSD) provides information on the 3D aspects of the present minerals. See chapter 6. When the CSD data is in 1D, it will be transformed to 2D and then to 3D. When the CSD data is in 2D, it will be transformed to 3D (using CSD corrections Higgins 2010). A fourth, optional input is the chemical composition of the source rock. This can be in element or oxide form and may contain only the bulk or mineral chemical compositions as well. In the latter case, the modal mineralogy can be retrieved from the chemical composition data.

1.3.3 Mineral properties

The properties of all input minerals and possible output minerals will be stored here. It consists of chemical properties, physical properties and inter-mineral properties. (i) The chemical properties include molar volume, molar mass, mineral formula and weathering rates. All except the latter are fixed properties, meaning that they will be retrieved from literature and will not change during running the model. The weathering rate of a mineral may be influenced by pH, temperature and relief (see boundary conditions). (ii) The physical properties are a mineral's strength and its density. The former plays a role in intra-crystal breakage (see mechanical weathering). (iii) The 'inter-crystal properties' have been separated from the previous 'intra-crystal properties' because they relate to properties between different crystals (of possible different mineralogy). Interface strength is the main property here, and will play a role in the inter-crystal breakage during mechanical weathering.

The intra- and inter-crystal strengths may be dependent on many factors such as anisotropies in crystal structure changes due to changes in temperature or pressure. A detailed approach to estimate the absolute strengths may be considered as building a model on its own and will thus be estimated here for time-efficiency reasons. The data of Heins (1992) may prove valuable here for estimating relative inter-crystal strengths while intra-crystal strengths may be gathered from literature. Notwithstanding these data, a more detailed approach could be argued here, and may be incorporated in the future. The modular architecture of SedGen will allow for such an adaptation.

See chapter 9.

1.3.4 Boundary conditions

The boundary conditions cover climate and physiography. (i) Climate governs temperature, pH and precipitation, all of which have an influence on chemical weathering rates. A general water availability model could also be incorporated in future work to better assess these influences. (ii) Physiography consist of the relief (in source area) and plays a role in both weathering processes. The general trend here is thus 'time' vs. intensity.

See chapter 10.

1.3.5 Mechanical weathering

The pre-processed input data are combined with the mineral properties and boundary conditions during the calculations of the mechanical weathering (as they will with the chemical weathering and clay formation modules). First, the source rock is broken into large rock fragments during 'intra-rock breakage'. A detailed mass balance is not accounted for these fragments, only their number and size. This can be argued because their compositions will be very similar to the initial conditions. When a large fragment, upon further abrasion, gets below a certain fractionation limit threshold, the detailed mechanical weathering kicks in. If a rock fragment is to be broken, inter-crystal breakage will be applied while if it concerns a (mono-mineralic) grain, intra-crystal breakage will be triggered. Bookkeeping by the mass balance of all grains and rock fragments becomes very important now for further developments of the system (see mass balance module).

See chapter 12.

1.3.6 Chemical weathering & precipitation

Grains and rock fragments resulting from mechanical weathering will be available for chemical weathering and thus will be dissolved. These solutes may remain in this state or may precipitate as authigenic minerals such as oxides or clays. Clay minerals can again be chemically weathered and re-enter the system in doing so.

See chapter 13.

1.3.7 Mass balance

The mass balance keeps track of all mono crystalline grains, poly crystalline grains (rock fragments), solutes and clay/oxides. The poly crystalline grains are further subdivided in mono mineralic and poly mineralic rock fragments. The accounting is done according to a Lagrangian framework, meaning that where the parts are present in the system is not relevant, only how many (and in which form) of each part is. For the mono crystalline grains a matrix of grain size classes and number frequencies per mineral is sufficient. For the polycrystalline grains a same matrix with number frequencies and grain size classes is combined with a separate matrix with rock fragment sizes.

1.3.8 Output

Output data consists of grains size distributions, mineralogy and grain number frequencies in the form of the accounting done in the mass balance module. The output of data can be requested (at any time?) by the user to zoom in on output at a specific time step.

1.3.9 Post-processing

Output data may be post-processed to generate time-evolution figures such as trajectories on ternary diagrams e.g.

CHAPTER **2**

Manual

2.1 Tips and Tricks

2.1.1 Image on the cover page

If you want to place an image on the cover of the dissertation, you can add the code underneath to the template (check with your promotor whether this is allowed).

Include image: Search for the `\frontcoverheaderXII` command in the `adsphd.cls` file and add the following lines:

```
\begin{textblock*}{56mm}(10mm+#1,15mm)
\includegraphics[width=56mm,height=20mm]{image/filename}
\end{textblock*}
```

Where 56mm is the width, 20mm the height, 10mm the x-location and 15mm the y-location.

Change cover font color: Add the command `\color{red}` to the `\frontcoverheaderXII` command or enclose specific parts. For example, `{\color{red}\textbf{\@authorf\ \@authorl}`.

2.1.2 Full cover page

Important: most printing services will create their own cover page based on the details you send them (title, name, affiliation, ...) and do not supply you with all necessary parameters (e.g., thickness of the paper) because these differ from machine to machine. Therefore, the generated cover page is only indicative and probably not used by your printing server (or even correct).

A full cover page (combining front cover, spine and back cover) can be generated automatically using the command `make cover` or `python3 run.py cover`. This creates a pdf `$(COVERPDF);` by default this is `cover.pdf`.

The width of the spine is set by redefining
`adsphdspinewidth` (9mm by default).

It can be seen in the provided `thesis.tex` that all information necessary to generate a cover page is contained between two markers

```
%%% COVER: Settings %%%
...
%%% COVER: End settings %%%
```

DO NOT REMOVE THESE!! They are used by the Makefile!!

The default front and/or back cover page can be overwritten:

- create a file `mycoverpage.tex`
- redefine the commands `\makefrontcovergeneral` and `\makebackcovergeneral`. For an example and more information, see the provided file `mycoverpage.tex`.

The cover page in the generated pdf has the following structure:

```
<--rbleed--><--backcoverpage--><--lbleed--><--spine width--><--lbleed--><--frontcoverpage--><--rbleed-->
```

The default bleed (both lbleed and rbleed) is 7mm. I suggest not changing this value unless you know what you are doing ;) The latter can be done by redefining `\defaultlbleed` and `\defaultrbleed` respectively.

2.1.3 Table of contents

To remove list of figures, tables and other preface chapters from the table of contents, search for occurrences of `\addcontentsline` in the file `adsphd.cls` and comment them.

2.1.4 Small ebook size

When you add the `epub` option to the adsphd class the dissertation is printed to a smaller size to read on a device such as Kindle.

Environments such as tables or tikZ pictures are often sized in absolute values and not relative to the size of the output. You can wrap them in a resizebox to enforce scaling:

```
\resizebox{\textwidth}{!}{%
  \begin{tabular}{cc}
    ...
  \end{tabular}
}
```

2.2 Settings for TeXstudio

If you are working with TeXstudio or other windows latex editors you might want to adjust the editor's settings to allow a proper compilation of the table of contents and list of figures/tables.

2.2.1 Custom *makeindex* and *makeglossaries* commands

According to the *README.md* the tables are indexed through two custom commands. To edit them in TeXstudio open the *Commands* settings (*Options* → *Configure TeXstudio...*, *Commands* sheet), edit the following fields and press OK.

Makeindex:

```
"C:/Program Files/MiKTeX 2.9/miktex/bin/x64/makeindex.exe" %.nlo -s nomencl.ist -o %.nls
```

Makeglossaries:

```
"C:/Program Files/MiKTeX 2.9/miktex/bin/x64/makeindex.exe" %.glo -s %.ist -t %.glg -o %.gls
```

Now the customized commands can be launched by using *Tools* → *Commands* → *MakeIndex/Makeglossaries*. If you want to automatize it in the standard *Build & View* (F5) and *Compile* (F6) commands look at the following section.

2.2.2 Custom Build&View and Compile meta-commands

Open *Options* → *Configure TeXstudio...*, *Build* sheet, edit the following field and press OK.

Build & View:

```
txs:///pdflatex | txs:///bibtex | txs:///makeglossaries | txs:///makeindex |
txs:///pdflatex  | txs:///pdflatex
```

To view the PDF once created you have to press F7 (or *Tool* → *View*) and the PDF will automatically update in the default viewer whan you modify it.

If you prefer to directly view the created PDF **from the beginning** edit the field as follow:

```
txs:///pdflatex | txs:///bibtex | txs:///makeglossaries | txs:///makeindex |
txs:///pdflatex  | txs:///pdflatex | txs:///view-pdf
```

Part I

Input

CHAPTER **3**

Dataset

This chapter will discuss the inside and outside of the Heins (1992) dataset which has been used and expanded throughout this PhD.

CHAPTER **4**

Modal mineralogy

...

CHAPTER **5**

Crystal boundary interfaces

...

CHAPTER **6**

Crystal size distributions

...

CHAPTER **7**

Parent rock characterization and initialization

...

CHAPTER 8

Input based on modified GGD

This chapter will discuss how the modified Generalized Griffiths' Descriptor (GGD) can be used to characterize a parent rock and be used as input for the model.

CHAPTER **9**

Mineral properties

...

CHAPTER **10**

Boundary conditions

...

Part II

Calculations/Implications/Algorithms

CHAPTER **11**

SedGen: design and architecture

11.1 Design guidelines

SedGen should be written in a popular programming language. The code base should be easily maintainable, while also being in some sort of version control system. A modular structure of the code base is also preferable.

11.2 Programming language

SedGen is written in Python and uses as main packages: numpy, pandas, matplotlib, etc. . All of these packages are widely used throughout the scientific community.

- Python is easy to use
- Python is low-level

CHAPTER **12**

Mechanical weathering

. . .

CHAPTER **13**

Chemical weathering

...

Part III

Applications

CHAPTER **14**

Calibration

...

CHAPTER **15**

Applications

...

CHAPTER **16**

Discussion

...

CHAPTER **17**

Conclusions

...

Instructies van de faculteit:

Algemene besluiten: Verwijzend naar de inleiding en naar de besluiten van de afzonderlijke hoofdstukken worden op het einde van het proefschrift de voornaamste besluiten gebundeld. Hier wordt de nadruk gelegd op de eigen inbreng, de verworven resultaten, de ‘stellingen’ van het proefschrift en de originele bijdragen tot het onderzoeksdomein. De onopgeloste problemen worden aangestipt en suggesties voor eventueel verder onderzoek worden gemaakt.

APPENDIX **A**

Appendix

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Instructies van de faculteit:

De appendices: ze omvatten alle gedeelten uit de tekst die weliswaar essentieel zijn voor het proefschrift, maar waarvan de inlassing in de tekst de leesbaarheid ervan nadelig zouden beïnvloeden bv. omwille van hun lengte. Zo kunnen bv. de brute meetresultaten of een computerprogramma met zijn bron, commentaar en voorbeelden beter thuishoren in een appendix dan in de tekst zelf. De appendices kunnen desgevallend worden gebundeld in een apart boekdeel.

Bibliography

Griffiths, J. (1952). "Grain-size distribution and reservoir-rock characteristics". In: *AAPG Bulletin* 36, pp. 205–229.

– (1961). "Measurement of the properties of sediments". In: *The Journal of Geology* 69, pp. 487–498.

Higgins, M. (2010). "Imaging birefringent minerals without extinction using circularly polarized light". In: *The Canadian Mineralogist* 48.1, pp. 231–235.

Instructies van de faculteit:

De bibliografie. Departementale richtlijnen terzake te volgen.

Curriculum

...

Instructies van de faculteit:

Beknopt CV van de doctorandus.

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Publications

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