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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

August 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.

Bram Paredis
Herent, August 2020

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

De vorming van sediment is een nog ondermaats onderzochte tak binnen de sedimentpetrologie.

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.

List of Abbreviations

GGD Generalized Griffiths Descriptor. 5

Contents

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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 is the research field in which one tries to understand how parent rock generates sediment along a specific pathway.

Parent rock is the rock from which the entire sediment generation process starts from. The properties of such a parent rock already limit the possible outcomes of the final sediment. Therefore, a proper way of characterizing the parent rock and thus its properties should be applied.

The **pathway** looks at by which processes sediment generation occurs, and along with it to which degree each process effects the outcome. Mechanical and chemical weathering are the major two groups with regard to the outlook of a pathway.

The properties of the resulting **sediment** is also of major interest.

1.2 General remarks

- In all relevant chapters parts of the SedGen model classes/functions/objects/constructs/ scripts may be included in the text or referenced as in appendix or online.
- Always note what we are and what we are not implementing into the model ⇒ Things can always be improved later on due to SedGen's modularity.

1.3 Chapter outline

1. Introduction
2. Input
   (a) Dataset
   (b) Generalized Griffiths Descriptor (Paredis et al. 2020)
   (c) Modal mineralogy (Weltje & Paredis 2020)
   (d) Relative interface frequencies (Weltje et al. 2018)
   (e) Crystal size distribution (Paredis et al. 2020)
3. SedGen model
   (a) SedGen architecture
   (b) Mechanical weathering
   (c) Chemical weathering and clay formation
4. Applications
   (a) Calibration
   (b) Post-processing + applications/test
   (c) General discussion and perspectives
5. Conclusions

1.4 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).

1.5 Model architecture

1.5.1 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.

1.5.2 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. (ii) The relative interface frequencies contain the fractions of all present mineral interface occurrences. See chapter 4. (iii) The crystal size distribution (CSD) provides information on the 3D aspects of the present minerals. See chapter 5. 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.

1.5.3 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 8.

1.5.4 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 9.

1.5.5 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 11.

1.5.6 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 12.

1.5.7 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.

1.5.8 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.

1.5.9 Post-processing

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

Part I

Input

CHAPTER **2**

Dataset

2.1 Chapter contents

- Introduction to main data set of Heins (1992): Geological setting of different plutons, number and identity of samples, etc. .
- Introduction to three main 'building blocks' of modal mineralogy, relative crystal interfaces and CSD

2.2 Data from literature

2.2.1 Data from Heins (1992)

The PhD thesis of Heins (1992) was the main source for data of this project. Since it holds detailed data on the mineralogical composition and texture of six granitoid plutons it was very suited to serve as the starting point for this PhD. Later on, the available data would be extended by means of own data collection (see next section).

Table 2.1: Number of samples collected by Heins (1992) for parent rock (P) and sediment (C: coarse; M: medium; F: fine)

	P	C	M	F
AZ	15			
CA-NS	5			
CA-EW	6			
GR	10			
MT	8			
WA	4			

Granitoid plutons

Six plutons were sampled by Heins (1992) which resulted in ca. 50 thin sections of parent rock and ca. 150 sediment samples across three size fractions (see Table 2.1).

2.2.2 Additional data sources

Throughout the PhD, other sources for data of various forms has also been used. One worth noting here is the Vistelius et al. (1983) which was used for both the spatial variability of modal mineralogy and textural information studies. References to those may be found in the relevant chapters.

2.3 Own data

Additional data was gathered to elaborate the dataset already collected by Heins (1992). The main addition was the digital image analysis carried out over a period of four months. During this analysis, data on crystal size was collected of all available thin sections from Heins (1992).

CHAPTER **3**

Modal mineralogy[1]

3.1 Chapter contents

- Modal mineralogy as one of the building blocks for SedGen
- Spatial variation of modal mineralogy (Ordinary Kriging of PCA) based on Weltje et al. 2020

3.2 First building block / fundamental property

3.3 Spatial variation of modal mineralogy

[1]this chapter is in part based on G. J. Weltje et al. (2018). “Quantitative analysis of crystal-interface frequencies in granitoids: Implications for modelling of parent-rock texture and its influence on the properties of plutoniclastic sands”. In: *Sedimentary Geology* 375, pp. 72–85

CHAPTER **4**

Crystal boundary interfaces

4.1 Chapter contents

- Based on Weltje et al. 2018 publication

4.2 Second building block / fundamental property

4.3

CHAPTER **5**

Crystal size distributions

5.1 Chapter contents

- Based on Paredis et al. 2019a publication
- 2D/3D CSD data
- Ways to transform and correct legacy data from 1D to 3D

5.2 Simulation of cutting spheres to circles

5.3 Digital image analysis

5.4 Truncation

CHAPTER **6**

Parent rock characterization and initialization

6.1 Chapter contents

- Based on Paredis et al. 2019a publication
- Determination of texture in granitoids
- Interaction of the three building blocks discussed by Heins' (1992) dataset as a way to initialize and characterize parent rocks for SedGen
- Characterization of all plutons from Heins (1992) separately

6.2

CHAPTER **7**

Input based on modified GGD

7.1 Chapter contents

- Griffiths' descriptor for sediments
- Our translation of Griffiths' description for granitoids and parent rocks in general (discussion): i) modal mineralogy, ii) relative crystal interfaces, iii) crystal size distributions
- Mention the fact that we leave out orientation and shape properties but that these could be included in future versions of SedGen (part of discussion)

7.2 Griffiths' descriptor

7.2.1 Griffiths' descriptor for sediments

7.2.2 Generalized Griffiths' descriptor (for parent rocks)

7.2.3 Fundamental properties of composition, texture and size

Composition - modal mineralogy

Texture - relative crystal interfaces

Size - Crystal size distributions

7.2.4 Remark on fundamental properties of shape and orientation

CHAPTER **8**

Mineral properties

8.1 Chapter contents

- Overview of physical and chemical properties of minerals
- Partly based on Weltje et al. 2020 with regard to relative interface strengths (inter-crystal properties)

CHAPTER **9**

Boundary conditions

9.1 Chapter contents

- Climate (temperature, pH, precipitation)
- Physiography (relief)
- Weathering rates (time vs intensity) → Alex Blum (reference)

9.2 Climate

Climatic conditions also have a role to play in the sediment generation process. **Temperature** and **precipitation** are the two most obvious factors. The **pH** of water can also be of importance when chemical weathering is the main form of weathering (e.g. solubility of K-feldspar).

9.3 Physiography

The **relief** of the terrain in which the sediment generation is occurring must also be taken into consideration. Along with the present **vegetation**, both will have an effect on mechanical and chemical weathering.

9.4 Weathering rate

All the factors mentioned in the above sections boil down to have a combined effect on the **rate of weathering**, be it mechanical or chemical.

Part II

Calculations/Implications/Algorithms

CHAPTER **10**

SedGen: design and architecture

10.1 Chapter contents

- General overview of how data should be formatted to be accepted by the model and the modules at work to clean, transform and calculate data in the case of legacy data.
- Types of weathering and their interaction
- Types of crystals/grains within SedGen (poly, mono, RF. . .)
- Discuss their implementation into the SedGen model and how they are tracked
- Different frameworks that are used in SedGen (e.g. Lagrangian framework, compositional space vs physical space)
- Discuss data that SedGen model can output and at what timesteps (GSD, mineralogy, grain number frequencies)

10.2 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.

10.3 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 **11**

Mechanical weathering

11.1 Chapter contents

- Based on Paredis et al. 2019b publication in which state-of-the-art in mechanical weathering will be discussed
- Since this field is less discussed in the geological literature, literature from others research fields will be consulted
- Discuss the mechanical weathering module of SedGen
- Intra- & inter crystal breakage along with intra-rock breakage in early stages of simulation (fractionation limit)
- Rock fragments on-demand

CHAPTER 12

Chemical weathering

12.1 Chapter contents

- State-of-the-art in chemical weathering and clay formation research
- Discuss sources from which information was implemented into the SedGen model
- Discuss the chemical weathering and clay formation modules of SedGen

Part III

Applications

CHAPTER **13**

Calibration

13.1 Chapter contents

- Discuss the validity of SedGen based on the calibration results of Heins (1992) and unseen test dataset

CHAPTER **14**

Applications

14.1 Chapter contents

- Provide a non-exhaustive list of possible applications of SedGen output data based on post-processed data (e.g. ternary diagrams, timestep based plots)

CHAPTER 15

Discussion

15.1 Chapter contents

- Discuss the applicability of SedGen in general
- Possibilities to upgrade SedGen due to its modularity (e.g. of including shape and orientation properties to input)

CHAPTER **16**

Conclusions

16.1 Chapter contents

- General conclusion of the current version of SedGen

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.

Appendices

APPENDIX **A**

Appendix

A.1 Chapter contents

- Additional figures
- Most important SedGen code snippets
- GitHub page reference for complete model code

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.

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Weltje, G. J., B. Paredis, L. Caracciolo, and W. A. Heins (2018). “Quantitative analysis of crystal-interface frequencies in granitoids: Implications for modelling of parent-rock texture and its influence on the properties of plutoniclastic sands”. In: *Sedimentary Geology* 375, pp. 72–85.

Instructies van de faculteit:

De bibliografie. Departementale richtlijnen terzake te volgen.

Curriculum

Bram Paredis was born in Neerpelt on July 6th, 1992. After completing his Latin-sciences studies at WICO Campus Sint-Hubertus in Neerpelt he started his academic studies at KU Leuven in 2010. There, he obtained his B.Sc. degree in Geology in 2013, followed by his M.Sc. degree in Geology in 2015. His M.Sc. thesis, which was supervised by Prof. Dr. Philippe Muchez, entitled 'Concentration and distribution of platinum group elements in sulfide ores: Musongati, Burundi' won the 'From Silex to Chip' prize awarded by the 'Beroepsvereniging Leuvense Geologen'. After receiving a negative advice for his application of a PhD grant to continue his petrology research, he made the switch the sediment petrology under supervision of Prof. Dr. Gert Jan Weltje where he started a PhD. Bram presented the results and outcomes of this PhD on numerous occasions. Bram has developed a strong interest for programming and data science in particular.

Instructies van de faculteit:

Beknopt CV van de doctorandus.

Publications

Journal papers

Weltje, G.J. and **Paredis, B.**, 2020. Spatial variability of modal mineralogy in granitoid plutons. Earth-Science Reviews xx, pp. xx-xx

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Miscellaneous

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