

Biologically-oriented mud volcano database: muddy_db

Alexei Remizovschi 1, Rahela Carpa Corresp. 2

Corresponding Author: Rahela Carpa Email address: rahela.carpa@ubbclui.ro

Mud volcanoes (MVs) are naturally occurring hydrocarbon hotbeds with continuous methane discharge, contributing to global warming. They host microbial communities adapted to hydrocarbon oxidation. Given their research value, MVs still represent a niche topic in microbiology and are neglected by hydrocarbon-oriented research. All the data regarding MVs is sporadic and decentralized. To mitigate this problem, we built a custom Natural Language Processing pipeline (muddy_mine), and collected all the available MV data from open-access articles. Based on this data, we built the muddy_db database. The muddy_db represents the first biologically oriented database rendered as a user-friendly web app. This database includes all the relevant MV data, ranging from microbial taxonomy to hydrocarbon occurrence and geology. The muddy_mine and muddy_db tools are licensed under the GPLv3.

muddy db R Shiny web app: https://muddy-db.shinyapps.io/muddy_db/

muddy_db R package: https://github.com/TracyRage/muddy_db

muddy_mine Conda package: https://github.com/TracyRage/muddy_mine

¹ Department of Molecular Biology and Biotechnology, Faculty of Biology and Geology, Babes-Bolyai University, Cluj-Napoca, - Select -, Romania

² Department of Molecular Biology and Biotechnology, Faculty of Biology and Geology, Babes Bolyai University, Cluj-Napoca, - Select -, Romania



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- Remizovschi Alexei¹ and Rahela Carpa¹
- ¹Department of Molecular Biology and Biotechnology, Babes-Bolyai University,
- Cluj-Napoca, Cluj, Romania
- Corresponding author:
- Rahela Carpa¹
- Email address: rahela.carpa@ubbcluj.ro

ABSTRACT

Mud volcanoes (MVs) are naturally occurring hydrocarbon hotbeds with continuous methane discharge, contributing to global warming. They host microbial communities adapted to hydrocarbon oxidation. Given their research value, MVs still represent a niche topic in microbiology and are neglected by hydrocarbon-oriented research. All the data regarding MVs is sporadic and decentralized. To mitigate this problem, we built a custom Natural Language Processing pipeline (muddy_mine), and collected all the available MV data from open-access articles. Based on this data, we built the muddy_db database. The muddy_db represents the first biologically oriented database rendered as a user-friendly web app. This database includes all the relevant MV data, ranging from microbial taxonomy to hydrocarbon occurrence and geology. The muddy_mine and muddy_db tools are licensed under the GPLv3. muddy_db R Shiny web app: https://muddy-db.shinyapps.io/muddy_db/

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INTRODUCTION

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Mud volcanoes (MVs) represent hydrocarbon discharging landforms (Mazzini and Etiope, 2017). They are distributed worldwide in both marine and terrestrial environments (Milkov, 2000). The most distinctive feature of MVs is recurrent methane emission. Due to methane emissions, MVs contribute extensively to global warming (Etiope et al., 2009).

MV genesis is mainly caused by a naturally mediated process - kerogen maturation (Vandenbroucke and Largeau, 2007). Therefore, the surrounding area of MVs can provide valuable data regarding both aerobic and anaerobic hydrocarbon microbial oxidation (Cheng et al., 2012).

Over the years, MVs research has been mainly focusing on anaerobic oxidation of methane (AOM) and the implicit interaction between sulfate-reducing bacteria and methane oxidizing archaea (ANME) (Bose et al., 2013; Cui et al., 2014). In addition to AOM research, MVs were also investigated in the context of hydrocarbon research. A myriad of MV studies discussed the thermogenic and biogenic origin of the methane (Etiope et al., 2009; Sano et al., 2017).

Despite these studies, the biological aspect of MVs is still a niche and unexplored topic. The biological data regarding MVs are sporadic and mostly biased towards AOM. Even worse, the already available data is not centralized. Due to the lack of the MV-dedicated database, researchers still analyze MV as a singular entity and avoid comparative studies between MVs with geographically distinct locations.

Meanwhile, mainstream biomedical fields have extensively employed natural language processing (NLP) techniques to mine meaningful data from the research articles (Wang et al., 2020). Simultaneously, the number of databases related to biomedical fields is considerable (Luo et al., 2016). Niche environmental science fields have not caught up. Lacking the possibility to mine environmental-oriented articles and build field-specific databases delays the publication of the meta-analyses or any comparative studies.

Fortunately, democratic NLP models and tools have been published over the last years. Some of them can be easily used by environmental scientists with limited computer science (CS) experience,



for example, the spaCy library, ScispaCy models, and S2ORC database (Honnibal and Johnson, 2015; Neumann et al., 2019; Lo et al., 2020).

Cumulatively, the latest advancements in NLP can provide opportunities for consolidating and promoting niche environmental topics such as MV microbiology.

Given these facts, we built the first biologically oriented mud volcano database, muddy_db, a niche database that consolidates all the relevant biological data, which will be of great use for researchers specializing in bacterial hydrocarbon oxidation or MV microbiology. Collaterally, our custom pipeline can serve as a methodological blueprint for research collectives interested in NLP and building their own specialized databases.

METHODS

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To collect all the available data regarding the biological aspects of MVs, we had to exclusively rely on open-access articles. Having these articles, we could freely mine all the biologically oriented tokens, including taxonomy-, chemicals-, geology-, and MV-specific terms. Additionally, we built a custom mining pipeline - muddy_mine (Fig. 1). The scope of muddy_mine is to provide and enrich the muddy_db database with relevant MV data.

Data collection

We used the S2ORC (20200705v1) database to collect open-access articles. S2ORC represents a centralized database that includes 12.7 million articles with a fully preserved paper structure. S2ORC is quite comprehensive and includes niche environment science articles (Lo et al., 2020). Given these facts, we extracted all the available MV-related titles (N=118 total, N=115 deduplicated) from the S2ORC.

Token extraction and muddy_mine pipeline

Having MV articles, we proceeded with token extraction (i.e. the extraction of the terms of interest) using the muddy_mine pipeline.

Taxonomy extraction represented a difficult challenge due to the fact that we intended to collect as many tokens as possible. To overcome this problem, we used the spaCy library (2.3.2), third-party ScispaCy NLP models (0.3.0), and the most recent NCBI Taxonomy database (20 November, 2020) (Honnibal and Johnson, 2015; Neumann et al., 2019; Schoch et al., 2020). First, we extracted all the taxon tokens using en_core_sci_sm ScispaCy model (2.2.5). Second, we checked those tokens against a local NCBI Taxonomy database. Third, we counted the extracted tokens. The higher the counting number, the more likely the token was explicitly discussed in the article.

By interating this third-step algorithm, we managed to centralize MV-specific taxonomy on all the possible levels: phylum, class, order, family, and genus.

The other non-taxonomy tokens were also extracted with the above-mentioned algorithm, We extracted and counted the tokens related to the following categories: chemistry (inorganic ions, hydrocarbons), geology (geological periods, minerals), MV terminology (ANME, methanogenesis type), and experimental methods (PCR types, amplified genes, chromatography). The comprehensive list of categories can be consulted by visiting the muddy_db repository.

The raw output of the muddy_mine pipeline represents a set of csv tables with MV data.

Building muddy_db database

By obtaining muddy_mine raw output, we can advance to the next step - building a user-friendly database. To create this kind of database, we created a Shiny web app, entitled muddy_db. In order to build it, we used the following R packages: shiny (1.5.0), semantic.dashboard (0.2.0), and golem (0.2.1) (Filip and Igras, 2021; Chang et al., 2021; Fay et al., 2021). This app includes all the output generated by the muddy_mine pipeline. Specifically, it displays the counted tokens extracted both from the integral article bodies (N=57) and abstracts (N=115). Additionally, we added an annotated map, which displays the geographical distribution of MVs and their affiliated research metadata.

System requirements

We would like to mention that muddy_mine pipeline was designed to run on systems with modest memory requirements. We achieved this feature by using Python generators. Intel Core i3 (3rd Gen) 3217U / 1.8 GHz processor (Intel, USA) and 4GB RAM system was used to build muddy_db. The mining process lasted 24 h.



RESULTS

The scope of the muddy_db is to gather all the available MV biologically relevant data and include it in a user-friendly database (Fig. 2). First, we collected all the known taxa associated with MVs.

The muddy_db includes data regarding archaeal and bacterial taxonomy on all the possible taxonomy levels. This particularity can facilitate the detection of microbial consortia patterns. Second, we gather information regarding metabolic pathways, geology, hydrocarbon availability, and experimental methods performed on MV sediments (Fig. 3). This information can guide specialists to implement appropriate research strategies.

DISCUSSION

MVs are considered to be one of the settings where the early life evolved (Pons et al., 2011). They sustain a plethora of bacterial metabolic pathways, ranging from methane oxidation and synthesis to sulphate reduction (Kleindienst et al., 2014; Cheng et al., 2012). These pathways and their affiliated microbial communities could provide valuable data regarding (1) origin of microbial life, (2) the effect of the naturally occurring methane discharging systems on global warming, (3) the contribution of microbial consortia to oil souring (Gieg et al., 2011; Etiope et al., 2009; Pons et al., 2011) As we can see, the accumulation of MVs data could enhance our knowledge regarding topics that range from fundamental studies to ecology and engineering.

Given these facts, MVs should be the main focus of hydrocarbon-oriented research and ecology. Unfortunately, data regarding the biological aspects of MVs are scarce. Additionally, the data already gathered are not combined in a dedicated database. The lack of a specialized MV database determines mud volcano microbiology to be a niche and neglected topic in environmental science.

Biomedical fields have always represented the cutting-edge subset of natural science, which actively implement CS techniques, and are tightly intertwined with the big data term (Luo et al., 2016). Simultaneously, the implementation of CS methods in niche environmental fields lags. To both apply CS methods in an environmental context and chronically mitigate the data deficient field of MV microbiology, we created a muddy_mine NLP pipeline and muddy_db database.

The creation of muddy_db tools aims to create a platform, that would provide sufficient data to perform meta-analyses or comparative studies of the MVs. Specifically, we hope that muddy_db would facilitate the discovery of atypical taxonomic patterns and point out the influence of geography on MVs characteristics. Simultaneously, muddy_mine represents a reproducible example of a mining technique applied in the context of environmental studies. As a result, muddy_mine could encourage researchers to mine their data of interest, being free from any field of study constraints.

In addition to positive sides of our projects, we would like to address the evident limitations of muddy_mine pipeline. We were limited to only to open-access articles which were found in the S2ORC. Currently, we are constricted to this corpus due to the following facts:

- 1. Journals use various article xml encoding standards such as TEI-XML and JATS-XML. Therefore, it is difficult to design a universal xml to json parser. As a result, it is challenging to manually create an exhaustive list of structured texts, which are appropriate for the mining process.
- 2. Unlike the open-access articles, the mining of articles behind the paywall might represent copyright infringement risks.

CONCLUSIONS

The muddy_db represents the first biologically oriented mud volcano database. It was designed to provide a comprehensive data corpus that can facilitate mud volcano research and shed light on the topic as a whole. The muddy_db contains data ranging from taxonomy to geology and experimental methods. Simultaneously, the muddy_mine NLP pipeline can serve as an example of accessible implementation of NLP techniques in environmental sciences.

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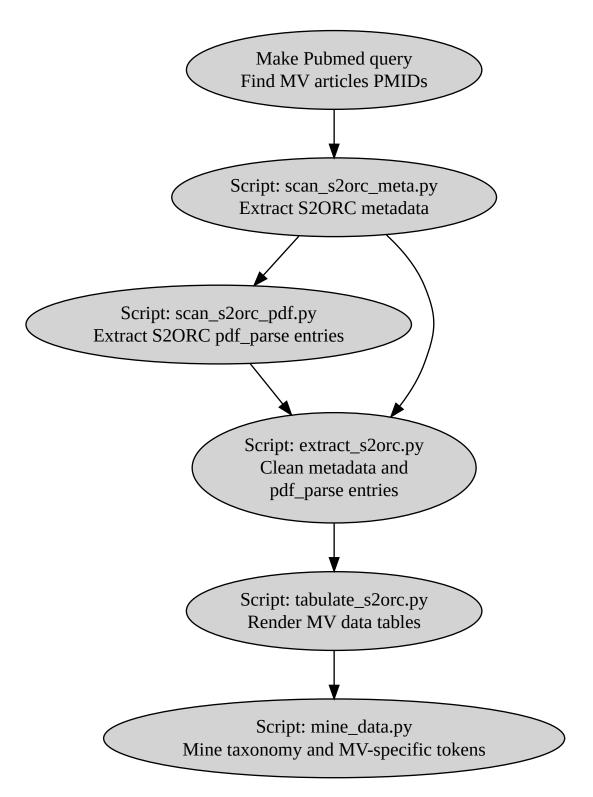


Figure 1. muddy_mine - pipeline used to build the muddy_db database. MV - mud volcano, PMIDs - Pubmed



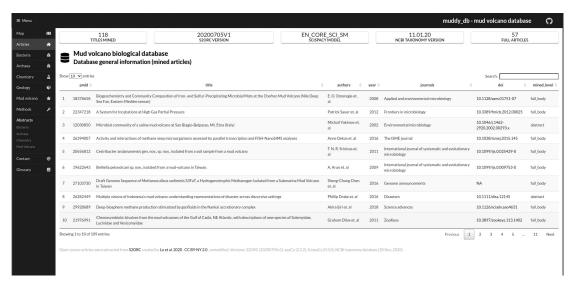


Figure 2. muddy_db general appearance

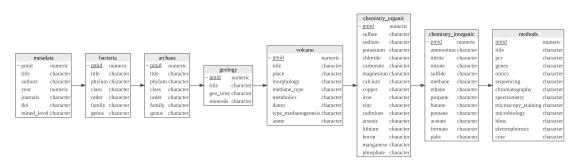


Figure 3. muddy_db schema