SedWeather: A Dashboard Package to Visualize Chemical Weathering of Clastic Sediments

For a provenance study and characterization of different types of sedimentological processes that affect weathering, chemical weathering of sediments is critical. We can estimate major elements of sedimentary geochemistry by using the various Weathering Indices (WIs) models. The present study is a fair attempt in the development of a web dashboard – SedWeather to analyze chemical weathering of sediments using major elemental geochemistry. It offers a flexibility to constrain sediments and rock composites and to demonstrate weathering profiles & source rock chemical makeup in various compositional space diagrams including Al2O3 – CaO-Na2O – K2O, Al2O3 – CaO-Na2O-K2O – Fe2O3-MgO, M – F – W; illustrates different various Weathering Indices (WIs) including CIW, CPA, CIA, PIA, CIX, ICV, WIP and W in boxplots, scatter matrix, correlation matrix against major oxides and ratios. It is possible to alter the Python code in accordance with the data and user requirement by altering the arguments and adding more relevant charts and plots to fit the data. SedWeather's performance in evaluating chemical weathering is demonstrated in evaluating sediments of Surma and Barail sandstones, Mizoram Foreland Basin, NE India, sediments of Manasbal Lake, Kashmir, India, and channel sediments, overbank sediments, suspended sediments of the Ganga basin, having their own provenance history.

**Keywords:** dashboard, geochemical provenance, Python, sediment weathering, weathering indices

# Introduction

To determine provenance, evaluate paleoclimates and tectonic activity, and to understand how the crust evolved, sedimentary rocks should be examined for their mineralogical and bulk chemical components [1–21]. Sedimentary rocks have been investigated in several studies for their mineralogy and bulk chemistry [4, 14, 18, 22–27]. It is vital to understand how sedimentary processes are responsible for producing sediments and how they affect them. Weathering, erosion, hydraulic sorting, and abrasion are some of these processes.

As Python's unique benefits have become more apparent in the Earth sciences community, it is gaining more users. "Early adopters" have no longer been the only ones adopting Python in Earth sciences. Graphs and charts can be easily understood as well as numbers and math. Data analytics doesn't always have to be difficult. It's not surprising that dashboards are widely used due to their ability to present complex stats in an understandable way. Geoscientific community is also not untouched with the advantages of dashboards. The use of dashboards is also helping in real-time interactive data visualization e.g., Indonesian Tsunami Early Warning System, glider scientific missions in the Gulf of Mexico recently [28, 29].

In the present study, we propose a dashboard package - SedWeather for evaluating chemical weathering of sediments and of rock composites containing major elements and oxides. To gain insight into the weathering profile and extent of rock alteration due to sedimentary processes, a Python programming environment has been used to develop a computer program that computes various weathering indices and several compositional space diagrams. This program also makes it easy to set argument and function values according to user requirements.

# MATERIALS AND METHODS

The dashboard app extends the possibilities of traditional "dashboards" by giving users a point-and-click interface for Python models [30]. SedWeather analyzes major elementals composition using python programming environment and helps in data storytelling using Dash.

## SedWeather

SedWeather follows a typical flowchart ([Fig. 1: flowchart](file:///F:\PhD%20Stuff\Project%20and%20Publication%20template\Scopus%20Indexed\Free\Evaluating%20Chemical%20Weathering%20of%20Sediments%20using%20Python\Figure\Flowchart.svg)), initiating with the installation and import of the necessary packages, through data loading, Weathering Indices (WIs) calculation & their statistical parameters to constrain data in various compositional space diagrams design. SedWeather initiates with the installation (optional) and import of required packages for performing required subsequent operations. Loading data in the relevant (‘csv’) format (as used for input in [Appendix: A-1](file:///F:\PhD%20Stuff\Project%20and%20Publication%20template\Scopus%20Indexed\Free\Evaluating%20Chemical%20Weathering%20of%20Sediments%20using%20Python\Appendix\sedchem.csv)), it calculates various chemical weathering indices (WIs) and generate different compositional space diagrams. Subsequently it provides statistical measures of weathering indices and their correlation with Al2O3/TiO2 using boxplots, scatter matrix, correlation matrices and correlation diagrams along with related data tables. Besides as required, user-defined variation plots of desired oxide/weathering index can also be visualized in the dashboard. All the generated tables (in ‘csv’ format) and plots (in ‘html’ format) get auto-stored in the parent directory. Additionally, the user can also get the plots downloaded in the vector (‘svg’) and raster (‘jpeg’) format (uncommenting a couple of lines in the code). SedWeather, coded in python programming environment (python 3.8.8) in a jupyter notebook ([Appendix: A-2](file:///F:\PhD%20Stuff\Project%20and%20Publication%20template\Scopus%20Indexed\Free\Evaluating%20Chemical%20Weathering%20of%20Sediments%20using%20Python\Appendix\SedWeather.ipynb)), follows the calculations of various chemical weathering indices and generates relevant tables & plots ([Fig. 2: layout](file:///F:\PhD%20Stuff\Project%20and%20Publication%20template\Scopus%20Indexed\Free\Evaluating%20Chemical%20Weathering%20of%20Sediments%20using%20Python\Figure\Layout.tif)). SedWeather code, compiled input data of major oxides composition and output plots & tables are made available in a public repository ([weblink](https://github.com/vinthegreat84/geochemistry/tree/master/SedWeather)) located in GitHub. The user is recommended to explore the repository for complete understanding of code, input data and generated plots & tables. However, only a few selected tables and plots are included in the present manuscript.

## Packages used

Packages are essential elements of Python, providing functions that help programmers avoid rewriting codes from scratch. SedWeather requires only a couple of commonly used python packages, thus does require only a basic level understanding of python and the packages used in the current study. As an open-source library for Python data manipulation, Pandas provides fast performance. As Pandas are based on Numpy, Numpy is required to operate. Dash is developed by Plotly, as well as a platform for writing Dash apps that can be deployed easily. SedWeather utilizes the inherited properties of these packages to analyze major elemental composition of sediments and rock composites.

## Input Data

For input data of SedWeather, rock composites of upper continental crust, [19, 31–39], igneous composites [40, 41], shales (PAAS - Post Archaean Australian Shale, NASC - North American shale composite, [42]; Shale, [43]; average Indian Archean Shale and average Indian post-Archean Shale {± Error at 95% Confidence Level}, [44], river sediments, denudation regions [45] and a few major elemental compositions (Manasbal Lake, [46]; Surma Group, Barail Group, [47]; channel sediments, overbank sediments, suspended sediments of Banas, Betwa, Chambal, Ganga, Ken, Sindh, Son, Ton, Yamuna rivers [48]; Silty\_clay, Sand of Meghna river, [49] from a variety of geological setting are considered.

Major oxide composition of clastic fines is taken from various rivers along with the average composition of DSDP fines of erosional products from major denudation regions of the world [45]. Lake sediments represent bottom sediments of warm, monomictic Mansabal lake in the kashmir valley, having with no major inflows. The distribution of sediments and chemical composition correlates well with the catchment lithology of carbonate bedrock & Panjal Traps and the associated sedimentary processes pointing towards shorter transport coverage and low sediment recycling. Surma and Barail sandstones belong to the Oligocene and Miocene periods of the Mizoram Foreland Basin, NE India. River sediments geochemistry represents major peninsular rivers of the Ganga basin including Yamuna, Ganga, Chambal, Sindh, Betwa, Ton, Ken, Son rivers. Meghna river composition represents silty clays and sand of one of the major rivers in Bangladesh, due to the rising Himalayas, carrying huge terrigenous, biogenous clastics to the adjacent ocean [49].

Input data is categorized into major oxides composition of category - composite (subcategory: upper\_continental\_crust {subsubcategory: UCC}; igneous\_composite {subsubcategory: ultramafic, mafic, intermediate, felsic}; shale\_composite {subsubcategory: shale}; river\_sediment {subsubcategory: suspended\_sediment}; region {subsubcategory: denudation}; and category - sample (subcategory: Manasbal\_Lake {subsubcategory: lake\_bottom}; Surma\_Group, Barail\_Group {subsubcategory: sandstone}; channel\_sediments, overbank\_sediments, suspended\_sediments {subsubcategory: Banas, Betwa, Chambal, Ganga, Ken, Sindh, Son, Ton, Yamuna}, Silty\_clay, Sand {subsubcategory: Meghna}.

Major oxides include (SiO2, TiO2, Al2O3, Fe2O3, FeO, MnO, MgO, CaO, Na2O, K2O, and P2O5) along with CO2 (wherever available) ([Appendix – A1](file:///F:\PhD%20Stuff\Project%20and%20Publication%20template\Scopus%20Indexed\Free\Evaluating%20Chemical%20Weathering%20of%20Sediments%20using%20Python\Raw\sedchem.csv)). Similar data template may be imported in the SedWeather web application framework for the user-defined composition to execute the code and to obtain relevant tables and plots.

## Chemical Weathering Indices and Compositional Space Diagrams

SedWeather calculates commonly used chemical weathering indices to evaluate and visualize the chemical weathering of clastic sediments. The indices included in the present study are:

* Chemical Index of Weathering [50]

CIW = Al2O3×100 / (Al2O3+CaO\*+Na2O) (1)

* Chemical Proxy of Alteration [51]

CPA = Al2O3×100 / (Al2O3+Na2O) (2)

* Chemical Index of Alteration [14]

CIA = Al2O3×100 / (Al2O3+CaO\*+Na2O+K2O) (3)

* Plagioclase Index of Alteration [52]

PIA = (Al2O3−K2O)×100 / (Al2O3+CaO\*+Na2O−K2O) (4)

* Modified Chemical Index of Alteration [53]

CIX = Al2O3×100 / (Al2O3+Na2O+K2O) (5)

* Index of Compositional Variability [5]

ICV = (Fe2O3+K2O+Na2O+CaO\*+MgO+MnO+TiO2) / Al2O3 (6)

* Weathering Index of Parker [54]

WIP = 100[(2Na2O/ 0.35) + (MgO/ 0.9) + (2 K2O/0.25) + (CaO\*/ 0.7)] (7)

* W index [55].

Besides, it also generates the plots of input data in various compositional space diagrams used to quantify chemical weathering of clastic sediments including A - CN - K compositional space diagram [14], M - F - W compositional space diagram [55], A - CNK - FM compositional space diagram [56].

## Boxplots and Correlation of Weathering Indices

Displaying the data quartiles (percentiles) and averages in a box plot visualizes the distribution and skewness of numerical data. SedWeather provides boxplot of chemical weathering indices for each subcategory (UCC, igneous\_composite, shale\_composite, suspended\_sediment, denudation\_regions, lake\_sediment, Surma\_sandstone, Barail\_sandstone). Scatter matrix of weathering indices helps understanding relationship with each other for lake\_sediment, Surma\_sandstone and Barail\_sandstone. Similarly correlation diagrams of weathering indices against Al2O3/TiO2 helpsestablishing correlations to visualize subtle changes in the chemical weathering. Additionally, the user is free to select any oxide/weathering index to generate a variation plot of the selected pair of variables, helping to explore quick correlations amongst oxides and weathering indices.

# Results and discussion

The output data table consists of the raw major elemental composition plus the calculated chemical weathering indices including CIW, CPA, CIA, PIA, CIX, ICV, WIP and W. [Table 1: WIs](file:///F:\PhD%20Stuff\Project%20and%20Publication%20template\Scopus%20Indexed\Free\Evaluating%20Chemical%20Weathering%20of%20Sediments%20using%20Python\Table\Calculated%20Weathering%20Indices%20(WIs)%20of%20sediments%20and%20rock%20composites.csv) displays the SedWeather calculated weathering indices of selected sediments and rock composites. Average CIA values ~70 of NASC and PAAS are in general agreement with reported values [14]. Similarly, calculated CIA average value ~51 of felsic suite is a close match [14]. Boxplot explains the CIA distribution and skewness characters of each subcategory ([Fig. 3: Boxplot of CIA variation](file:///F:\PhD%20Stuff\Project%20and%20Publication%20template\Scopus%20Indexed\Free\Evaluating%20Chemical%20Weathering%20of%20Sediments%20using%20Python\Figure\Boxplot%20of%20CIA%20variation.jpeg)). Median CIA value ~51 for upper continental crust and ~67 for shale composites fairly matches with the reported values [14, 44]. Calculated CIA values ~51 for the St. Lawrence River and ~95 for the Niger River explains the accuracy of SedWeather [45]. Lake sediment provides an average CIA value ~39 while Surma sandstone and Barail sandstone give CIA value ~35 and ~45 respectively [47]. However, W is calculated ~28, ~54, ~62 respectively for these compositions. Calculated weathering indices for rock composites including upper\_continental\_crust, igneous\_composite and shale\_composite are summarized in [Table 2: WIs of composites](file:///F:\PhD%20Stuff\Project%20and%20Publication%20template\Scopus%20Indexed\Free\Evaluating%20Chemical%20Weathering%20of%20Sediments%20using%20Python\Table\WIs_stats%20-%20Copy.xlsx).

Scatter matrix indicates a positive correlation amongst CIW, CPA, CIA, PIA, CIX and negative correlation amongst ICV, WIP, W for lake sediment ([Fig. 4: Scatter matrix of lake sediment](file:///F:\PhD%20Stuff\Project%20and%20Publication%20template\Scopus%20Indexed\Free\Evaluating%20Chemical%20Weathering%20of%20Sediments%20using%20Python\Figure\scatter%20matrix%20of%20weathering%20indices%20of%20Manasbal%20Lake.jpeg)). Similar relationship is observed for Surma sandstone and Barail sandstone ([Fig. 5: scatter matrix of Surma](file:///F:\PhD%20Stuff\Project%20and%20Publication%20template\Scopus%20Indexed\Free\Evaluating%20Chemical%20Weathering%20of%20Sediments%20using%20Python\Figure\scatter%20matrix%20of%20weathering%20indices%20of%20Surma%20Group.jpeg), [Fig. 6: scatter matrix of Barail](file:///F:\PhD%20Stuff\Project%20and%20Publication%20template\Scopus%20Indexed\Free\Evaluating%20Chemical%20Weathering%20of%20Sediments%20using%20Python\Figure\scatter%20matrix%20of%20weathering%20indices%20of%20Barail%20Group.jpeg)). Correlation diagrams express a positive correlation of CIW, CPA, CIA, PIA, CIX, ICV, W and a negative correlation of WIP with Al2O3/TiO2 for lake sediment ([Fig. 7: correlation of lake sediment](file:///F:\PhD%20Stuff\Project%20and%20Publication%20template\Scopus%20Indexed\Free\Evaluating%20Chemical%20Weathering%20of%20Sediments%20using%20Python\Figure\Correlation%20diagram%20of%20chemical%20weathering%20indices%20of%20Manasbal_Lake.jpeg)).

Major element composition of suspended sediment from major rivers and the erosional products from some major denudation regions of the world plotted in A-CN-K compositional space diagram ([Fig. 8: A-CN-K for rs\_r](file:///F:\PhD%20Stuff\Project%20and%20Publication%20template\Scopus%20Indexed\Free\Evaluating%20Chemical%20Weathering%20of%20Sediments%20using%20Python\Figure\UCC_rs_r%20plot%20in%20A%20-%20CN%20-%20K%20compositional%20space.jpeg)) is also plotted identically [45]. The plot clearly shows a consistent trend with a progressive increase in chemical weathering, thus affecting typical UCC composition. Besides, matching pattern of igneous rock suite is observed when plotted in M-F-W compositional space diagram ([Fig. 9: M-F-W for igneous](file:///F:\PhD%20Stuff\Project%20and%20Publication%20template\Scopus%20Indexed\Free\Evaluating%20Chemical%20Weathering%20of%20Sediments%20using%20Python\Figure\igneous_composite%20plot%20in%20M%20-%20F%20-%20W%20compositional%20space.jpeg)). UCC compositions plot in a restricted space in the ternary plots of A - CN - K compositional space, M - F - W compositional space and A - CNK - FM compositional space diagram ([Fig. 10: A-CK-K for UCC](file:///F:\PhD%20Stuff\Project%20and%20Publication%20template\Scopus%20Indexed\Free\Evaluating%20Chemical%20Weathering%20of%20Sediments%20using%20Python\Figure\upper_continental_crust%20plot%20in%20A%20-%20CN%20-%20K%20compositional%20space.jpeg), [Fig. 11: M-F-W for UCC](file:///F:\PhD%20Stuff\Project%20and%20Publication%20template\Scopus%20Indexed\Free\Evaluating%20Chemical%20Weathering%20of%20Sediments%20using%20Python\Figure\upper_continental_crust%20plot%20in%20M%20-%20F%20-%20W%20compositional%20space.jpeg), [Fig. 12: A-CNK-FM for UCC](file:///F:\PhD%20Stuff\Project%20and%20Publication%20template\Scopus%20Indexed\Free\Evaluating%20Chemical%20Weathering%20of%20Sediments%20using%20Python\Figure\upper_continental_crust%20plot%20in%20A%20-%20CNK%20-%20FM%20compositional%20space.jpeg)). Same goes correct for shale composites in the ternary plots of A - CN - K compositional space, M - F - W compositional space and A - CNK - FM compositional space diagram ([Fig. 13: A-CN-K for shale](file:///F:\PhD%20Stuff\Project%20and%20Publication%20template\Scopus%20Indexed\Free\Evaluating%20Chemical%20Weathering%20of%20Sediments%20using%20Python\Figure\shale_composite%20plot%20in%20A%20-%20CN%20-%20K%20compositional%20space.jpeg), [Fig. 14: M-F-W for shale](file:///F:\PhD%20Stuff\Project%20and%20Publication%20template\Scopus%20Indexed\Free\Evaluating%20Chemical%20Weathering%20of%20Sediments%20using%20Python\Figure\shale_composite%20plot%20in%20M%20-%20F%20-%20W%20compositional%20space.jpeg), [Fig. 15: A-CNK-FM for shale](file:///F:\PhD%20Stuff\Project%20and%20Publication%20template\Scopus%20Indexed\Free\Evaluating%20Chemical%20Weathering%20of%20Sediments%20using%20Python\Figure\shale_composite%20plot%20in%20A%20-%20CNK%20-%20FM%20compositional%20space.jpeg)). Lake sediment plots in a restricted space clustering towards FM apex in A - CNK - FM compositional space diagram ([Fig. 16: A-CNK-FM for lake](file:///F:\PhD%20Stuff\Project%20and%20Publication%20template\Scopus%20Indexed\Free\Evaluating%20Chemical%20Weathering%20of%20Sediments%20using%20Python\Figure\UCC_ml%20plot%20in%20A%20-%20CNK%20-%20FM%20compositional%20space.jpeg)) indicating low to average degree of chemical weathering of the catchment rocks with near similar composition to that the source rock. M - F - W compositional space diagram, plotting along M-F axis, indicates a granitic to granodioritic composition of sediments of Surma sandstone and Barail sandstone ([Fig. 17: M-F-W for sg\_bg](file:///F:\PhD%20Stuff\Project%20and%20Publication%20template\Scopus%20Indexed\Free\Evaluating%20Chemical%20Weathering%20of%20Sediments%20using%20Python\Figure\UCC_sg_bg%20plot%20in%20M%20-%20F%20-%20W%20compositional%20space.jpeg)). However, Surma sandstone seems more mafic in composition in comparison to the Barail sandstone when plotted in M - F - W compositional space diagram. Therefore, they seem to be sourced from different felsic source rocks. When peninsular river compositions of the Ganga basin are plotted in A - CN - K compositional space diagram, channel sediments form cluster near the feldspar line in contrast to the suspended sediments closer to the A apex. As expected, the overbank sediments are plotted between the suspended and the channel sediments ([Fig. 18: A-CN-K of Peninsular rivers of Ganga Basin](file:///F:\PhD%20Stuff\Project%20and%20Publication%20template\Scopus%20Indexed\Free\Evaluating%20Chemical%20Weathering%20of%20Sediments%20using%20Python\Figure\UCC_cs_os_ss%20plot%20in%20A%20-%20CN%20-%20K%20compositional%20space.jpeg)). It seems pointing to the control of weatherable source material in low relief, stable tectonic regime assisted by the subtropical climate condition [48]. As reported, river sediments of Meghna River display lower values of K2O, Na2O, and CaO as compared to UCC and do follow an ideal trend of weathering ([Fig. 19: A-CN-K of Meghna River](file:///F:\PhD%20Stuff\Project%20and%20Publication%20template\Scopus%20Indexed\Free\Evaluating%20Chemical%20Weathering%20of%20Sediments%20using%20Python\Figure\UCC_sc_s%20plot%20in%20A%20-%20CN%20-%20K%20compositional%20space.jpeg)). While silty clays show slightly more weathered composition as compared to sand, both of them form distinct clusters in M - F - W compositional space diagram close to F-W axis ([Fig. 20: M-F-W of sc\_s](file:///F:\PhD%20Stuff\Project%20and%20Publication%20template\Scopus%20Indexed\Free\Evaluating%20Chemical%20Weathering%20of%20Sediments%20using%20Python\Figure\UCC_sc_s%20plot%20in%20M%20-%20F%20-%20W%20compositional%20space.jpeg)), suggesting and supporting the argument of poor to average source weathering derived from felsic source rocks [49].

# Conclusion and future roadmap

With Python, one can write simpler and error-free code as its elegant syntax and extensive tool set assist earth scientists in writing less buggy code. Using basic understanding of python and dash, SedWeather may be customized further for the desired algorithms as required. The scope of current study includes production of data tables and plots of different chemical weathering indices. However, SedWeather may be modified further to include other geochemical aspects as well including normalized-plots, various bivariate diagrams, chemical classification diagrams, ratio plots, tectonic setting discrimination diagrams etc.

The following conclusions may be drawn for selected sediments as evaluated using SedWeather:

* Sandstone samples from the Surma Group, Mizoram Foreland Basin, seem to have been transported long distances and sorted by sediment type.
* Chemical weathering is moderately evident in the source terrain of the sandstones of the Surma Group and Barail Group.
* As far as chemical composition is concerned, Manasbal lake sediments show little or no chemical change with the major elements practically the same as those in the source rocks.
* By using compositional space diagrams, sandstones from the Mizoram Foreland Basin are believed to have originated from a felsic source rock in the Himalayan Foreland Basin.
* On the other hand, the sediments in Manasbal lake indicate a sediment source from basaltic components (Panjal traps and carbonate bedrock), controlled by the catchment lithology.
* Sediments from the Mizoram Foreland Basin and Manasbal lake show fundamentally different geochemical evolution and contrasting origin, indicating contrasting provenance.
* Peninsular river sediments of Ganga basin have witnessed varying intensities of chemical weathering and grain sorting due to their long-distance transport.
* Sediments of Meghna River have undergone poor to moderate level of chemical weathering of felsic source rocks along with grain sorting.

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# Appendix

A-1: sedchem: Compiled major oxides composition of category - composite (subcategory: upper\_continental\_crust {subsubcategory: UCC}; igneous\_composite {subsubcategory: ultramafic, mafic, intermediate, felsic}; shale\_composite {subsubcategory: North American shale composite, Post Archaean Australian Shale, Shale, Indian Archean Shale, Indian post-Archean Shale}; river\_sediment {subsubcategory: suspended\_sediment}; region {subsubcategory: denudation}; and category - sample (subcategory: Manasbal\_Lake {subsubcategory: lake\_bottom}; Surma\_Group, Barail\_Group {subsubcategory: sandstone}; channel\_sediments, overbank\_sediments, suspended\_sediments {subsubcategory: Meghna}, Silty\_clay, Sand {subsubcategory: Banas, Betwa, Chambal, Ganga, Ken, Sindh, Son, Ton, Yamuna}.

A-2: SedWeather: A web application framework to visualize Chemical Weathering of Clastic Sediments

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**List of Tables**

Table 1: Calculated Weathering Indices (WIs) of selected sediments and rock composites.

Table 2: Average Weathering Indices (WIs) of rock composites.

# List of Figures

Figure 1: Process flowchart of ‘SedWeather’ as scripted in python programming environment.

Figure 2: Execution flowchart of ‘SedWeather’ python program.

Figure 3: Boxplot of CIA variation for selected sediments and rock composites.

Figure 4: Scatter matrix of Manasbal lake sediment.

Figure 5 Scatter matrix of Surma Group sandstone.

Figure 6 Scatter matrix of Barail Group sandstone.

Figure 7: Correlation of different weathering indices with Al2O3 /TiO2 for Mansal lake sediments.

Figure 8: A-CN-K compositional space diagram of suspended river sediments and denudation regions.

Figure 9: M-F-W compositional space diagram of different igneous composites.

Figure 10: A-CN-K compositional space diagram of Upper Continental Crust (UCC) composites.

Figure 11: M-F-W compositional space diagram of Upper Continental Crust (UCC) composites.

Figure 12: A-CNK-FM compositional space diagram of Upper Continental Crust (UCC) composites.

Figure 13: A-CN-K compositional space diagram of different Shale composites.

Figure 14: M-F-W compositional space diagram of different Shale composites.

Figure 15: A-CNK-FM compositional space diagram of different Shale composites.

Figure 16: A-CNK-FM compositional space diagram of Mansal lake sediments.

Figure 17: M-F-W compositional space diagram of Surma Group and Barail Group sandstone.

Figure 18: A-CN-K compositional space diagram of Peninsular rivers of Ganga Basin.

Figure 19: A-CN-K compositional space diagram of Meghna river sediments.

Figure 20: M-F-W compositional space diagram of Meghna river sediments.