Theory and Application of the Python Program Frost-Cracking Intensity Calculator (FCIC)

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ABSTRACT

Frost-Cracking Intensity Calculator (FCIC; pronounced “F-kick”) was developed using the Python distribution, Anaconda, for the purpose of calculating frost-cracking intensity using the Hales and Roering method. This software utilizes multiple packages, including Tkinter, NumPy, Pandas, and Seaborn to help manipulate the data, build a simple graphical user interface, and output data for visualization or further manipulation in Excel. Using climatic data on a watershed-scale as input, FCIC calculates correct frost-cracking intensity data far more efficiently than Excel and may be web-based, thereby providing an easily accessible scientific tool.

1. INTRODUCTION

There is a plethora of geoscientific processes that could benefit from computerization with calculation of frost-cracking intensity being no exception. Because of the complexity of the mathematical calculations, the creation of frost-cracking intensity determination is difficult and tedious through Excel. A program would greatly facilitate this calculation and data manipulation while lowering the risk of human error. In addition, improved data visualization is offered through the Frost-Cracking Intensity Calculator (FCIC; pronounced “F-kick”).

The purpose of this paper is to showcase the creation, coding, capabilities, and calculated Python-based results of FCIC. Initially, the mathematical formalization of the FCIC will be presented, followed by the discussion of the programming language and packages used. The capabilities of FCIC will be demonstrated by analyzing the inputs, outputs, and graphical user interface. Finally, the outcome and results of the program will be evaluated to determine if FCIC achieves the desired solution of making frost-cracking intensity simple and easily calculated.

2. BACKGROUND

2.1 Mathematical Model

Frost-cracking intensity (FCI) is defined as the depth-integrated annual sum of the temperature gradient ($\partial t/\partial z$) which occurs in the frost-cracking window if 0 to -15 °C (Girard et al., 2013; Rempel et al., 2016). The FCI calculated herein utilizes the Hales and Roering (2007) method which works well at the watershed-scale and only requires climatic data and the thermal diffusivity of the bedrock.

Equation (1) calculates temperature (T) as a function of depth (*z*) in bedrock and time (*t*) using a one-dimensional heat conduction equation given a sinusoidal surface temperature variation (Anderson, 1998; Hales and Roering, 2007; Savi et al., 2015).

$$T(z,t) = MAT + Ta \times \exp\left[-z \times \left(\frac{\pi}{\alpha P_y}\right)^{0.5}\right] \times \sin\left[\frac{2\pi t}{P_y} - z \times \left(\frac{\pi}{\alpha P_y}\right)^{0.5}\right] \quad (1)$$

Where,

T(z,t) = Temperature as a function of depth (z) in bedrock and time (t)

MAT = Mean annual temperature

T_a = Half the amplitude of the sinusoidal variation, the difference between maximum summer and winter minimum temperatures

P_y = Period of one year

α = Thermal diffusivity of rock

Equation (2) provides the depth-integrated annual sum of the temperature gradient which occurs within the frost-cracking window of 0 to -15 °C (Girard et al., 2013; Rempel et al., 2016; Price et al., 2022).

$$\left|\frac{\partial T}{\partial z}\right| (°\mathrm{C cm}^{-1}) = \left|\frac{T(z_{i+1},t)-T(z_i,t)}{z_{i+1}-z_i}\right|, \mathrm{for}\ -15°\mathrm{C} \le T(z_i,t) \le 0°\mathrm{C} \quad (2)$$

Equation (3) is the formula for calculation of frost-cracking intensity (Price et al., 2022).

$$FCI\ (°\mathrm{C\ cm}^{-1}\mathrm{year}^{-1}) = \sum_{i=0}^{n}\sum_{t=1}^{Py}\left|\frac{T(z_{i+1},t)-T(z_i,t)}{z_{i+1}-z_i}\right|, -15°\mathrm{C} \le T(z_i,t) \le 0°\mathrm{C} \quad (3)$$

3. MATERIALS & METHODS

3.1 Language and Package Choice

Frost-cracking intensity was coded using the Python programming language, which handles data and its manipulation quite well. This especially true for scientific computations as it offers several packages and tools, and a robust collection of built-in data types (Millman & Aivazis, 2011). Specifically, Anaconda was used which is a distribution of Python designed for data science (Anaconda Software Distribution, 2016). Anaconda provides multiple packages applicable to the development of FCIC, but contained in a single package. The integrated development environment (IDE) used was PyCharm Community which is free and offers many benefits such as code completion, integrated debugging (JetBrains, 2017), and supports Anaconda and its many scientific packages (Anaconda Software Distributions, 2016). The multiple packages used in the creation of FCIC served different purposes such as data manipulation, data visualization, graphical user interface (GUI), and distribution.

3.2 Data Manipulation Packages

The data manipulation packages include NumPy, Pandas, and XLWings. NumPy offers efficient multidimensional arrays on which a variety of mathematical operations can be performed (Harris et al., 2020). This is useful for calculating FCI as thousands of values must undergo mathematical computations. Pandas is used to manipulate and structure data into two-dimensional DataFrames (McKinney et al., 2010). Similar to Excel tables, FCIC uses DataFrames to structure frost-cracking intensity data in a neatly ordered manner for keeping track of different data values. XLWings is an open-core spreadsheet interaction and automation package used to read and write to Excel files (XLWings, 2023). A large part of FCIC is outputting the data into an easily editable and further manipulatable format, in this case, Excel.

3.3 Data Visualization Packages

The Frost-Cracking Intensity Calculator utilizes Matplotlib and Seaborn for data visualization. Matplotlib is used to visualize and plot graphs of data (Hunter & J.D., 2007), whereas Seaborn is based on Matplotlib and goes a step further by providing high-level code to facilitate graphing. In addition, Seaborn is integrated with both NumPy and Pandas (Waskom et al., 2017), making it a great candidate to assist in the creation of FCIC.

3.4 Graphical User Interface and Distribution Packages

With respect to the GUI, FCIC uses the package Tkinter which is the standard package that simplifies interface creation (Lundh, 1999). Frost-Cracking Intensity Calculator only requires limited form-style inputs along with a few buttons, so Tkinter was adequate for the interface. For the distribution of FCIC, PyInstaller was chosen because it can bundle the whole application into a single package for distribution. While FCIC could operate on a website, a desktop-application option was chosen for the initial stages of this project.

3.5 Graphical User Interface Introduction

Frost-Cracking Intensity Calculator is relatively straightforward to use. It is divided into two inputs and outputs with the user entering the information requested and pressing the "Calculate FCI," button (Figure 1). All the parameters in the input section are required before FCI will be calculated otherwise an error message is displayed. With respect to the output section (lower box of display), the labels will remain blank until FCI is calculated, at which point they populate with the appropriate FCI values (Figure 1). Below the output boxes, two buttons offer additional options to the user. The left button exports the formatted results to an Excel file for further manipulation and/or viewing, and the bottom right button yields an interactive graph of

FCI vs. depth (Figure 1). The interactive GUI of the graph is provided by the Matplotlib package.

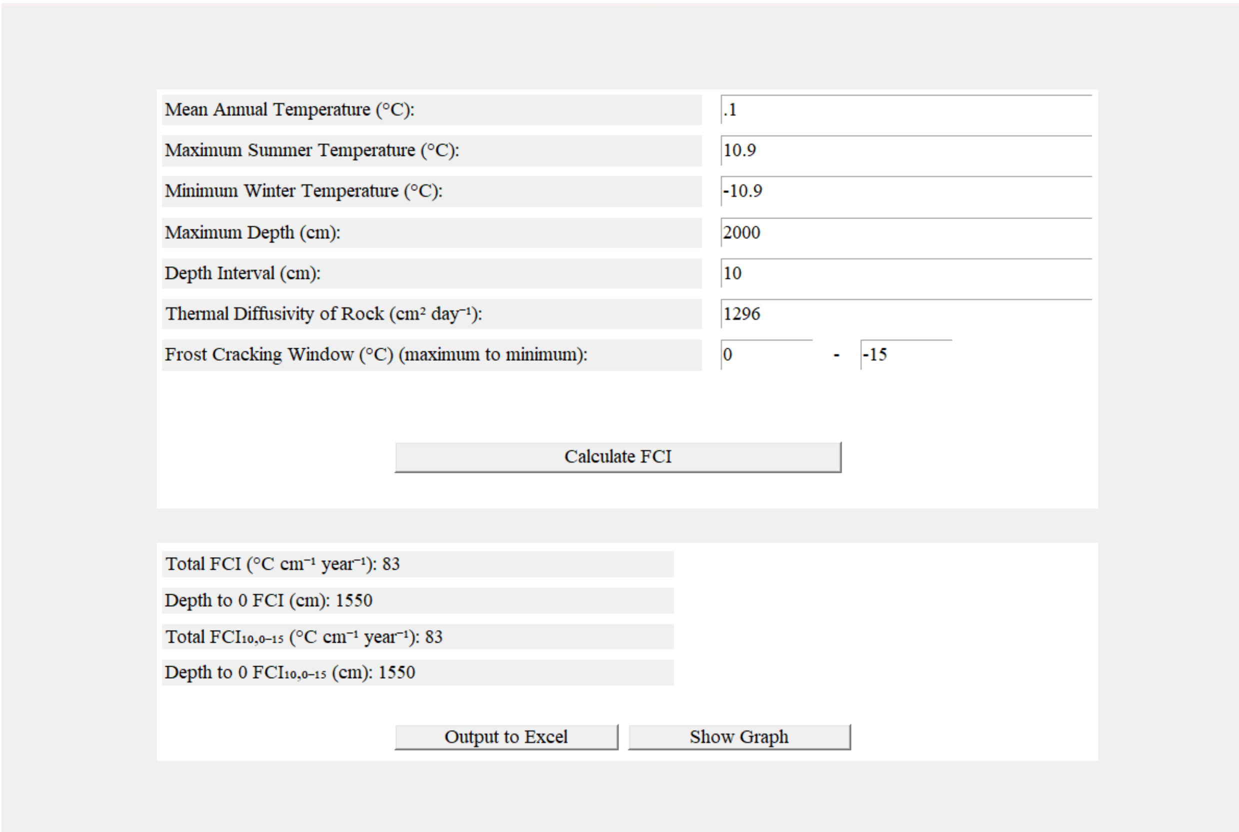

Figure 1. The graphical user interface for FCIC, consisting of the upper user input section and the lower calculated output section.

3.6 Input Data

Similar to the GUI, the input data required to run FCIC is relatively simple as follows:

- Mean Annual Temperature (°C)
- Maximum Summer Temperature (°C)
- Minimum Winter Temperature (°C)
- Maximum Depth (cm)
- Depth Interval (cm)

- Thermal Diffusivity of Rock (cm^2 day^{-1})
- Frost Cracking Window Maximum (°C)
- Frost Cracking Window Minimum (°C)

With the exception of the depth interval these inputs support decimal numbers. Frost-Cracking Intensity Calculator will also not accept invalid numbers such as negative depth or depth interval, and will produce an error message if the frost-cracking window is invalid. If and when any of these errors occur, FCI will not be able to be calculated.

3.7 Output Results

When the user selects the button to calculate FCI (assuming all parameters are correct), FCIC will compute and populate the output cells with: (1) The total FCI; (2) The depth at which FCI reaches zero for the user-defined depth interval and frost-cracking window; and (3) The normalized FCI depth interval to 10 cm and for a frost-cracking window of 0 to -15 °C (Figure 1). Additional information may be accessed through either of the two buttons below the output. The "Output to Excel" button creates an Excel sheet with the following data (for both user-defined and normalized FCI calculations) (Figure 2):

- Total annual FCI for the year (°C cm^{-1} $year^{-1}$)
- Mean annual temperature (MAT) (°C)
- Ta (half of the amplitude of the climatic sinusoidal variation) (°C)
- Maximum Depth of frost-cracking (cm)
- Depth interval (cm)
- Thermal Diffusivity of Rock (cm^2 day^{-1})
- Frost cracking window (°C)

- Depth at which FCI reaches 0 (°C cm^{-1} $year^{-1}$)

	A	B	C	D	E	F	G	H	I	J
1	Total FCI (°C cm^{-1} $year^{-1}$)	Total $FCI_{10;0-15}$ (°C cm^{-1} $year^{-1}$)	MAT (°C)	T_a (°C)	Max Depth (cm)	Depth interval (cm)	Thermal Diffusivity of Rock (cm^2 day^{-1})	Frost Cracking window (°C)	Depth to 0 FCI (cm)	Depth to 0 $FCI_{10;0-15}$ (cm)
2	83	83	0.1	5.45	2000	10	1296	0.0 - -15.0	1550	1550
3										
4										
5	Depth (cm)	FCI (°C cm^{-1} $year^{-1}$)		Depth (cm)	$FCI_{10;0-15}$ (°C cm^{-1} $year^{-1}$)					
6	0	2.24		0	2.24					
7	10	2.19		10	2.19					
8	20	2.13		20	2.13					
9	30	2.08		30	2.08					
10	40	2.02		40	2.02					
11	50	1.97		50	1.97					
12	60	1.92		60	1.92					
13	70	1.87		70	1.87					
14	80	1.83		80	1.83					
15	90	1.78		90	1.78					
16	100	1.73		100	1.73					
17	110	1.69		110	1.69					
18	120	1.65		120	1.65					
19	130	1.60		130	1.60					
20	140	1.56		140	1.56					
21	150	1.52		150	1.52					
22	160	1.48		160	1.48					
23	170	1.44		170	1.44					
24	180	1.40		180	1.40					
25	190	1.37		190	1.37					
26	200	1.33		200	1.33					

Figure 2. Frost-Cracking Intensity Calculator Excel output values.

The “Show Graph,” button launches the Matplotlib interactive GUI plotted with the user-defined data. The plot depicts frost-cracking intensity as a function of depth and allows the user to immediately view these results (Figure 3).

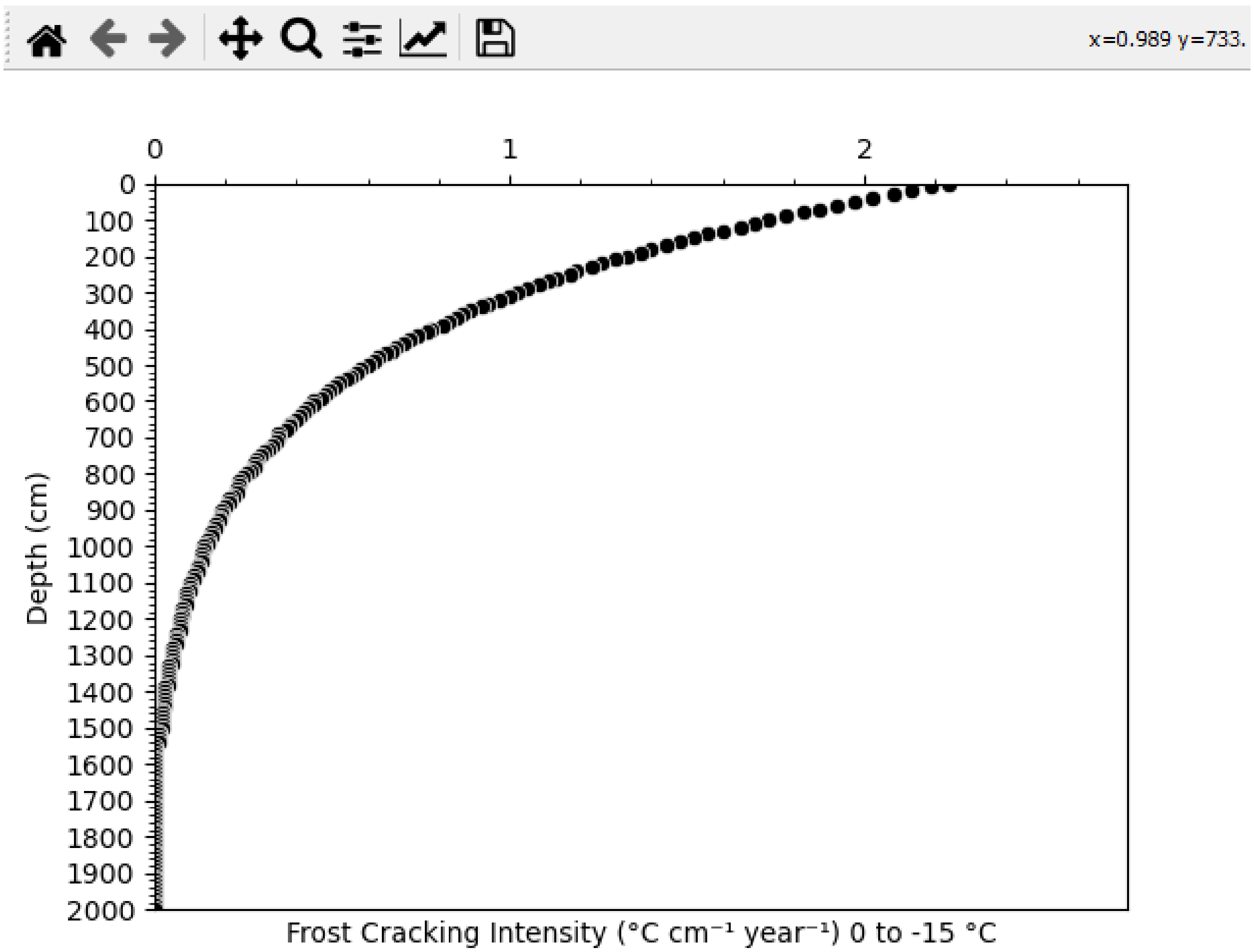

Figure 3. Graph visualization of frost-cracking intensity using GUI with example data.

4. RESULTS & DISCUSSION

4.1 Comparison of Results

Identical sample data input into both FCIC and an in-house prepared Excel spreadsheet yielded identical results. Though Excel permits greater control over the data, FCIC can handle the data much more efficiently while yielding identical results.

4.2 Advantages and Disadvantages of FCIC

Prior to the development of FCIC, calculating frost-cracking intensity was highly inefficient and tedious. Users would have to use software such as Excel to manually input the calculations to create and store thousands of data values and. In contrast, FCIC efficiently calculates more data, and more rapidly than Excel, while minimizing user effort. In addition, FCIC is much more intuitive, thereby minimizing error.

Although FCIC has many merits it does exhibit some limitations. This calculator was developed to only perform the Hales and Roering (2007) method of calculation, which primarily utilizes climatic data for application at the watershed-scale. Consequently, FCIC does not utilize more advanced methods of FCI calculation, such as for calculations applied to the outcrop scale (Draebing & Mayer, 2021). Another limitation is that FCIC is only available via a desktop application, not a web application. While this is not a serious limitation, it means that FCIC is somewhat less accessible from a distribution point of view. However, this issue can be addressed in a future project.

5. CONCLUSIONS

Frost-Cracking Intensity Calculator (FCIC) was developed to be a simple, convenient, and efficient scientific tool to calculate frost-cracking intensity in bedrock. By utilizing various data science software and packages, FCIC achieved this goal by minimizing user effort and manipulating large amounts of data. In addition, FCIC delivers faster and more enhanced data manipulation with the addition of exporting and visualizing data, both in Excel and Matplotlib's interactive graph GUI.

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