

Introduction to CharRec and model design considerations

CharRec is a spatially explicit computational model that simulates the formation of long-term charcoal records based on empirically supported models of primary charcoal transport (Fig. 1). The model is an exploratory tool that assists researchers in interpreting how natural and anthropogenic fire regime components contribute to the formation a sedimentary charcoal record. One of the most challenging aspects of developing computer simulations of social-ecological systems is including enough complexity to address specific research questions while reducing the amount of uncertainty in the model structure and parameters. Pattern-oriented modeling offers a strategy for optimizing the relationship between complexity and uncertainty by focusing on multiple patterns observed in real systems at differing scales (Grimm et al., 2005). Such models focus on a small number of underlying processes that can be calibrated independently to influence the overall pattern of the system (2005:989). CharRec does not attempt to capture the extensive complexity of charcoal production, dispersion, and deposition. Instead, it utilizes four specific components that contribute to the overall patterning of primary charcoal in sedimentary records. These include fire spatial distribution, frequency, size, and intensity. These characteristics are most susceptible to manipulation by humans, thus providing a means for testing the influence of burning practices related to land-use on the formation of charcoal records. A diagrammatic representation of CharRec is shown in figure 1.

The following section provides details regarding the specific modules that comprise CharRec and presents a statistical method for systematically comparing CharRec simulated charcoal data to empirical datasets. CharRec is built in Netlogo Version 6.0.3, an agent-based programming language and open-access modeling environment (Wilensky, 1999). Netlogo is ideal for this modeling application because it is easily programmed and customized, has a user-friendly interface, and the ability to couple with other open-access GIS and statistical software.

CharRec modules and main components

CharRec is composed of five modules, which include the 1) Landscape, 2) Ignition Scenario, 3) Burn, Disperse, and Deposit, 4) Form record, and 5) Export modules; together these simulate the formation of a sedimentary charcoal record on an annual time scale. In a simulation run, fires disperse micro- and macro-charcoal throughout the landscape, which is aggregated at a designated sampling point according to a set deposition interval (e.g., 100 years cm^{-3}). At the end of each deposition interval, charcoal counts are exported as a single observation in the charcoal record series. A diagrammatic representation of the relationship between CharRec modules is illustrated in Fig. 2.

1. Landscape module

The CharRec model landscape is a geo-referenced representation of a user-defined study area and is composed of rasters representing topographic, atmospheric, and fuel conditions. The physical terrain of the model landscape is represented by a raster digital elevation model (DEM) applied to each landscape patch. Atmospheric input rasters are created from modern local weather station measurements of wind velocity and direction. These data are interpolated across the model landscape using WindNinja, a free software program developed by the U.S Forest Service Rocky Mountain Research Station's Fire, Fuel, Smoke Science Program (Forthofer et al., 2014). WindNinja creates patch-specific, spatially varying wind fields based on topographic variation.

Fuels in CharRec are based on the 13 fuel models developed by Anderson (1982) for predicting wildfire behavior. Although updated models have improved accuracy in North American ecosystems (see Scott and Burgan, 2005), the original 13 models have been adapted to describe a diverse range of international ecosystems. For broad usability, CharRec uses these original models. Available dead and live biomass approximations for 1-hour and 10-hour fuel size classes are assigned to each landscape patch. Assuming an equal distribution of fuels across each patch, potential heat release rates from combustion are calculated for all fuel model size classes (Johansen et al., 1976: Equation 1) and used to approximate plume injection heights resulting from convective uplift (Clark, 1988a: Equation 5). These calculations are done assuming a wind velocity of 0 meters sec^{-1} , thus producing the maximum potential plume injection height for each fuel class. These data are saved in CharRec as global variables for later use in the Burn, Disperse, and Deposit module.

2. *Ignition Scenario module*

The Ignition Scenario module determines the fire regime components (fire spatial distribution, frequency, size, and intensity) used each model run. These variables are set by the user to simulate natural or anthropogenic ignitions and influence charcoal production, dispersion, and deposition in subsequent modules. To begin the module, fire frequency is determined annually by a Poisson probability distribution based on a user-defined mean-ignitions-per-year value (see Higuera et al., 2007 for a similar method). A low mean-ignitions-per-year value may result in many model years that do not have any fires burning on the landscape, while a higher value will allow for multiple fires to burn simultaneously.

Fire spatial distribution is determined by the ignition probability of each landscape patch. A random-number algorithm is used to determine a fire's potential location; this algorithm is weighted to favor areas with high ignition probabilities over those with low probabilities. The range of probability values available to the random-number algorithm is set by a user-defined probability cutoff. In practice, if the probability cutoff is set at 0, all landscape patches within the model landscape have the potential to ignite. If the probability cutoff is set at 0.5, a subset of landscape patches with ignition probabilities above or equal to 0.5 have the potential to ignite. The probability cutoff parameter allows for a range of spatial configurations to be tested.

Changes in fire size are modeled through a spread function that randomly selects the number of directly adjacent patches that a fire will spread to. The number of adjacent patches ranges from 0 to 8; a value of 0 indicates that a fire will remain in its original patch (0.09 ha), while a value of 8 indicates the fire will spread to all adjacent patches via a shared edge or a shared vertex (0.81 ha). Fire intensity of the original fire is assigned to all additional fires as it spreads.

Within CharRec, fire intensity refers to the amount of energy released from the combustion of fuels at each landscape patch (Keeley, 2009). Fuel size classes and plume injection heights calculated in the Landscape module are used to differentiate between fire intensities. For example, when an ignition scenario includes low-intensity fires, only plume injection heights calculated from the heat release rate of 1-hour fuels are used. Ignition scenarios with high-intensity fires use plume injection heights calculated from the heat release rate of both 1-hour and 10-hour fuels. Although there is variation within fuel models, generally a fire consuming 1-hour fuels results in a shorter plume injection height than a fire consuming both 1-hour and 10-hour fuels.

3. *Burn, Disperse, and Deposit module*

Once a fire ignites on a landscape patch, its intensity determines the size class of available biomass that is consumed and the injection height of the resulting plume. Available biomass is converted into charcoal mass using the conversion rate published by Gavin (2001:32). Charcoal mass is then transformed into micro- and macro-charcoal particle counts based on experimental charcoal particle size distribution data published by Pitkänen et al. (1999). Plume injection height for each fire is modified by wind velocity at the fire's patch following the empirical relationship illustrated by Clark (1988a: Equation 5). Finally, the amount of micro- and macro-charcoal dispersed at a given x and y distance from a fire's patch is calculated using a three-dimensional form of Clark's (1988a) Gaussian aerial transport model adapted by Peters and Higuera (2007: Equations 1 and 2). The equations are reproduced below (see Higuera et al., 2007 and Peters and Higuera, 2007 for Gaussian aerial transport model details and inputs):

$$\chi(x,y) = \frac{2vQ(x)}{u\pi C_y C_z x^{2-n}} \exp\left(\frac{-y^2}{C_y^2 x^{2-n}}\right) \exp\left(\frac{-h^2}{C_z^2 x^{2-n}}\right) \quad (1)$$

$$Q(x) = Q_0 \exp\left\{ \frac{4v_g}{nu C_z \sqrt{\pi}} \left[-x^{n/2} e^{-\xi} + \left(\frac{h}{C_z}\right)^{2m} \times \left(\Gamma(-m+1) - \Gamma_{\xi}(-m+1) \right) \right] \right\} \quad (2)$$

Micro- and macro-charcoal fallout occurs according to wind direction at the fire's origin. Counts of micro- and macro-charcoal are recorded only when fallout reaches and deposits charcoal at the user-designated sampling site. The Burn, Disperse, and Deposit module operates for every fire that burns on the model landscape during a model year.

4. *Form Record and Export modules*

Sediment accumulation rates in CharRec are determined by a user-defined deposition interval, which sets how many years represent one cubic centimeter of deposition. Once the number of model years in the deposit interval is reached, the Form Record module aggregates charcoal counts at the sample location into single observations of micro- and macro-charcoal. A complete CharRec simulation is run for a user-defined number of deposit interval observations. At the end of the simulation, the Export module collates all charcoal count observations created by the Form Record module, as well as ignition scenario variables used during the simulation, and exports them as a spreadsheet. A map of all fire locations created during the simulation is also exported in raster format.

5. *Statistical comparison of model outputs to an empirical charcoal record using LDA*

Linear discriminant analysis (LDA) is a statistical method for classification that reduces a dataset into a lower dimensional space while maximizing the separation between multiple classes (Duda et al., 2001). LDA is a flexible and robust classification technique that it does not require data standardization (i.e. z-score transformation) or normal distributions, making it an ideal candidate for comparing CharRec outputs to empirical sedimentary charcoal data. LDA uses an initial dataset to form linear combinations of predictor variables that emphasize differences between classification groups. The resulting linear discriminants can then be used to classify new data, generating posterior probabilities of classification group membership for each observation in the new dataset. The best-fit classification for each new observation is determined by the

highest posterior probability. The distribution of posterior probabilities for other classification groups provides insight into the quality of the best-fit classification.

When comparing CharRec simulated charcoal data to an empirical charcoal record, the unique ignition scenario parameters from each complete simulation constitutes a classification group. Linear discriminants for charcoal data created by CharRec are used to predict ignition scenario membership for each micro- and macro-charcoal observation in the empirical dataset. The ignition scenario with the highest posterior probability is considered a ‘best-fit’ for a given observation in the empirical dataset. Prediction quality for the best-fit ignition scenario is assessed by comparing its posterior probability to the mean probability of all classification groups in the original dataset; the greater a best-fit ignition scenario’s deviation from the mean posterior probability, the higher its prediction quality.

Installing R extension for Netlogo and special considerations for Windows users

The R extension for Netlogo is a vital component of CharRec and must be installed prior to running any simulations. If the R extension is not installed, Netlogo will produce an error. To install the R extension for Netlogo, please follow the instructions at for all operating systems at <https://ccl.northwestern.edu/netlogo/docs/r.html>. Once the R extension is installed, the user must select the location of the R script containing the plume dispersion model when setting up CharRec. To do this, press “1. R code”. This will open a file folder dialog where you can navigate to the R code included with the CharRec download folder. Select this code and continue with the set-up steps.

*****Windows Users:** All steps of the installation instructions for the R extension provided by Netlogo must be followed exactly, otherwise the extension will not function properly. Please follow the additional steps that are not currently outlined in the Netlogo guide for the R extension:

Specify the location where R is storing installed packages:

- a. Open the user.properties file (located in "C:\Program Files\Netlogo 6.0.3\app\extensions\r") and locate the r.home and jri.home.paths lines that should have already been edited if following the R extension installation instructions.
- b. Beneath these lines is another line that is commented out, that starts with “r.lib.paths”. This is how the r extension finds the paths to installed libraries in R.
- c. Uncomment this line and replace all of the text after the “=” with the path to the current R libraries. It should be similar to this, but with the user’s Windows profile username instead of <current-user>: "C:/Users/<current-user>/Documents/R/win-library/4.1
- d. Save the user.properties file and restart Netlogo. If having trouble saving the user.properties file due to permissions restrictions, one option around this is to drag the file to the desktop, edit it, then drag it back into its original folder.

Citing the model

Please use the following citation when referencing CharRec:

Snitker, G., 2018. Identifying natural and anthropogenic drivers of prehistoric fire regimes through simulated charcoal records. *Journal of Archaeological Science* 95, 1–15. <https://doi.org/10.1016/j.jas.2018.04.009>

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Figure 1: Diagrammatic representation of CharRec modules

