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Supplementary Material

BARA: cellular automata simulation of multidimensional smouldering in peat with horizontally varying moisture contents

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Appendix

BARA: Cellular Automata Simulation of Multidimensional Smouldering in Peat with Horizontally Varying Moisture Contents

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A. Supplementary figures

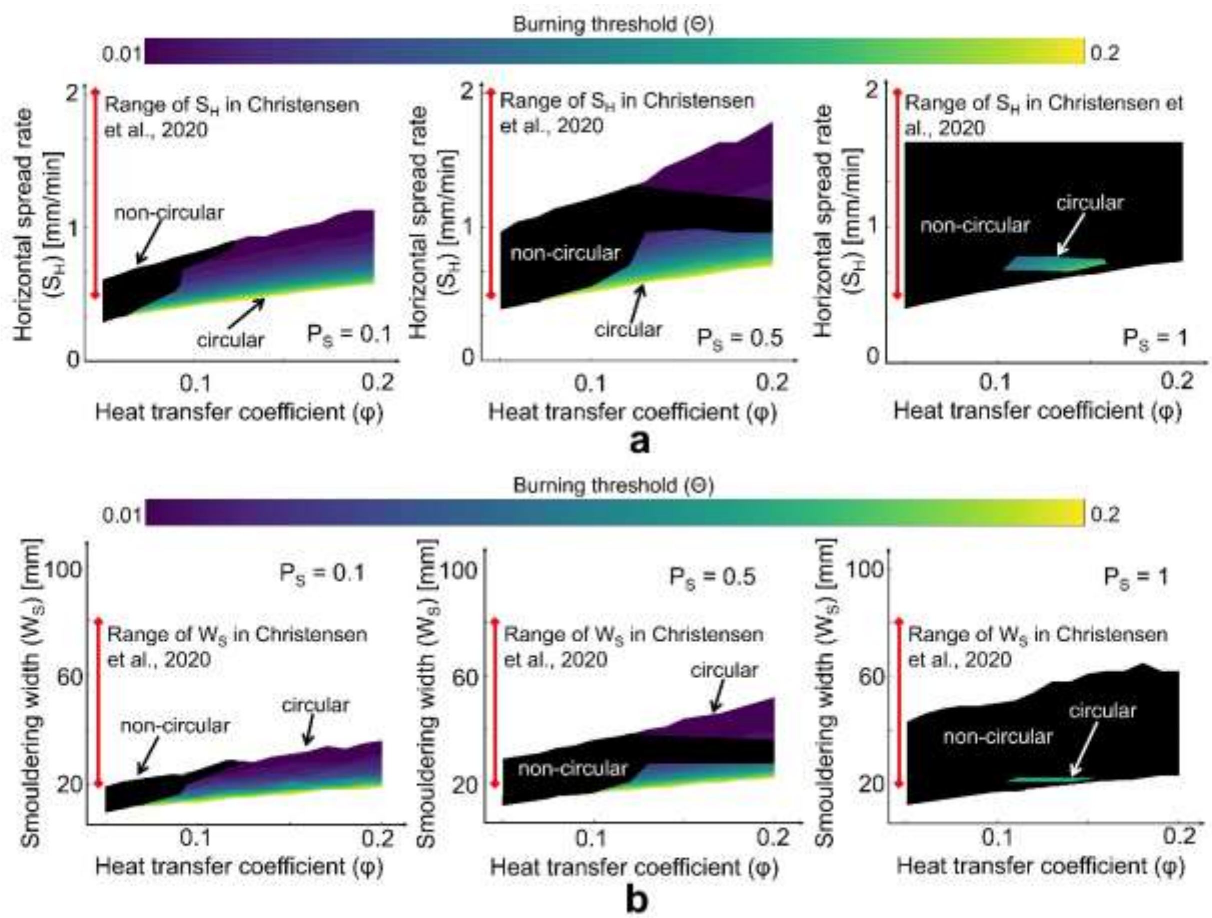

Figure A1. Sensitivity analysis of P_s on different Θ and φ based on (a) horizontal spread rate (S_H) and (b) smouldering width (W_S). Regions shaded in black represent simulations with non-circular shape (unexpected results).

B. Derivation from first principle

Heat release rate

Fig. 3 illustrates consumed peat at one time-step and its components. Consumed peat with the volume of ($\delta V = \Delta x^2 \delta$) contains water with a volume of δV_w, inorganic content with a volume of δV_i, air with a volume of δV_a, and organic content with a volume of δV_o. The heat release rate (Q_R) depends on the heat generation per m^3 (ΔH_c) and δV_o as shown in Eq. A1. By using mathematical operations, δV_o can be formulated as a function of organic density (ρ_o), particle density of the peat (ρ_o'), and δV. The thickness of the consumed peat is a function of vertical spread rate (S_d), therefore, Q_R can be formulated as shown in Eq. A6 where b_1 is a constant. By assuming constant ΔH_c, ρ_o' and Δx, Eq. A6 can be simplified to become Eq. 3.

$$Q_R = \Delta H_c \delta V_o \tag{A1}$$

$$\frac{\delta V_o}{\delta V} = \frac{\rho_b}{\rho_o'} \cdot \frac{m_o}{m_b} = \frac{1}{\rho_o'} \cdot \frac{m_o}{\delta V} \tag{A2}$$

$$\frac{\delta V_o}{\delta V} = \frac{\rho_o}{\rho_o'} \tag{A3}$$

$$Q_R = \Delta H_c \frac{\rho_o}{\rho_o'} \delta V \tag{A4}$$

$$Q_R = \frac{\Delta H_c}{\rho_o'} \rho_o \Delta x^2 \delta \tag{A5}$$

$$Q_R = \left(b_1 \Delta x^2 \frac{\Delta H_c}{\rho_o'}\right) \rho_o S_d \tag{A6}$$

Heat transfer coefficient

Fig. A2 shows the physical analogy of heat transfer in BARA and heat transfer in the physical term. If two adjacent cells have different heat values (H), this condition is analogous to having different temperatures (T) in physical term. Due to the temperature difference (ΔT), there is heat transfer (Q) from a cell with higher temperature (red) to a cell with lower temperature (blue). By assuming a 1D transient conduction heat transfer (Eq. A7) with effective thermal conductivity, k_e (see Eq. A8) for porous media following Huang *et al.* (2015), a finite difference method is applied to the Eq. A7 which results in Eq. A9. In these equations, T is temperature, t is time, ρ_b is bulk density, c is specific heat, x is distance, k is material thermal conductivity, Φ is porosity, γ is the radiative conductivity coefficient, and σ is the Stefan–Boltzmann constant. Meanwhile, ΔT_{1-2} is the temperature difference between cell 1 (west neighbour) and cell 2 (centre cell) and ΔT_{3-2} is the temperature difference between cell 2 and cell 3 (east neighbour). These equations are implemented in BARA where the heat transfer is discretized to one time step and to one neighbour (the other three sides of the cell are assumed to be insulated). Therefore, in Eq. A9, $\Delta t = 1$ and $\Delta T_{3-2} = 0$, resulting in Eq. A10 when the temperature is translated to heat value. These processes are repeated independently for the other three neighbours (in this example North, East, South), therefore, although the heat transfers between a centre cell and each neighbour are not directly connected, eventually they affect one another. This neighbourhood concept is one of the reasons CA becomes computationally efficient. To further simplify the model, k_e is set to be constant resulting in Eq. A11 where b_2 is a constant. In BARA, the heat value transferred to the neighbour (Q) is ${}^{\delta H}/_{\Delta l}$, where Δl is the number of cells that separate the two cells which are interacting. Therefore, Eq. A11 can be further modified to be Eq. A12 where φ is heat transfer coefficient in BARA which depends on the ρ_b and c of the sample.

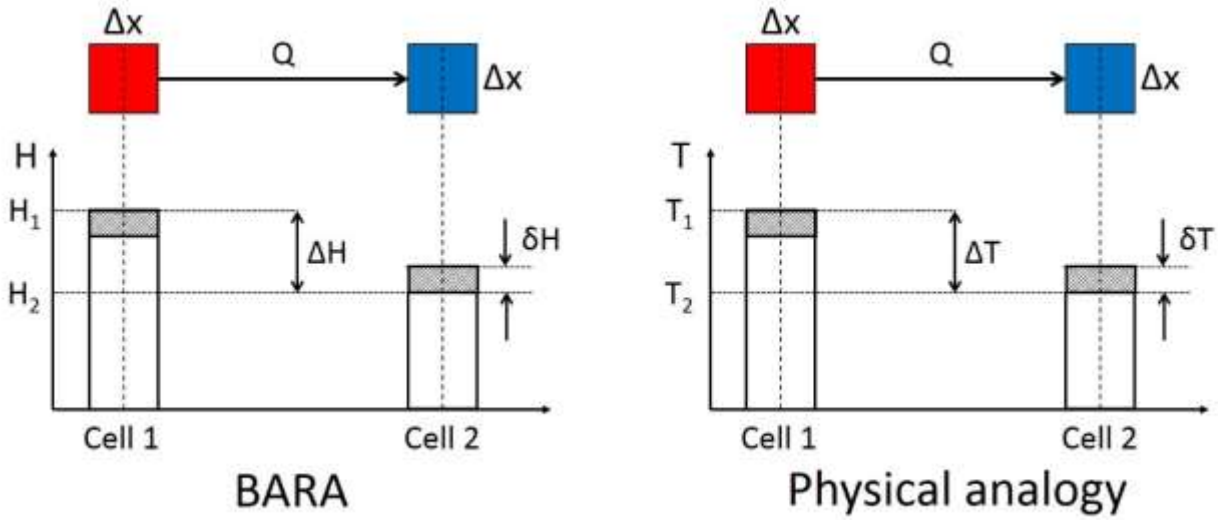

Figure A2. Schematic of analogy of heat transfer in BARA and physical analogy.

$$\frac{\partial T}{\partial t} = \frac{k_e}{\rho_b c} \cdot \frac{\partial^2 T}{\partial x^2} \qquad \text{(A7)}$$

$$k_e = k(1 - \Phi) + \gamma \sigma T^3 \qquad \text{(A8)}$$

$$\frac{\Delta T}{\Delta t} = \frac{k_e}{\rho_b c} \cdot \frac{\Delta T_{1-2} + \Delta T_{3-2}}{\Delta x^2} \qquad \text{(A9)}$$

$$\delta H = \frac{k_e}{\Delta x^2} \frac{\Delta H}{\rho_b c} \qquad \text{(A10)}$$

$$\delta H = \frac{b_2}{\rho_b c} \Delta H \qquad \text{(A11)}$$

$$Q = \varphi \frac{\Delta H}{\Delta l} \qquad \text{(A12)}$$