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Application of the Shuffled Complex Evolution Algorithm for Thermokinetic Parameter Identification in Fire Safety Engineering

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INTRODUCTION & AIM

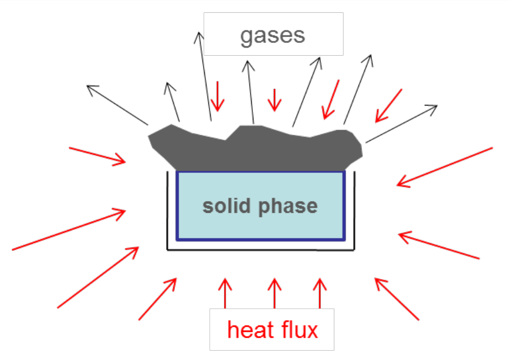
Fire safety engineering requires accurate thermokinetic parameters for pyrolysis modelling of building materials. Cone calorimeter tests measure the mass loss rate (MLR) as a function of time, a fundamental parameter in the fire behaviour study. Two natural bio-based insulation materials are studied: banana-fibre foam and flax-fibre foam. Determining material-specific parameters from experimental MLR curves is an ill-posed inverse problem requiring global optimization.

Aim

- Calibrate solid-phase pyrolysis model (15 parameters) for two natural insulation foams using cone calorimeter data
- Apply Shuffled Complex Evolution (SCE) as global optimizer to minimize discrepancy between simulated and experimental MLR
- Validate the parameter identification methodology and assess transferability to other bio-based materials

METHOD

Solid-Phase Pyrolysis Model



Definition of decomposition reaction equation number:

$$[A]_1 \rightarrow v_{s,1} \cdot [A]_2 + v_{H2O,1} \cdot [H_2O]_2 + v_{fuel,1} \cdot [HC]_2$$
$$[A]_2 \rightarrow v_{s,2} \cdot [A]_{k+2} + v_{H2O,2} \cdot [H_2O]_3 + v_{fuel,2} \cdot [HC]_3$$
$$\dots$$
$$[A]_{k+1} \rightarrow v_{s,k+1} \cdot [A]_{k+2} + v_{H2O,k+1} \cdot [H_2O]_{k+2} + v_{fuel,k+1} \cdot [HC]_{k+2}$$

Each single-reaction rate can be parameterized in terms of two major variables: the temperature, T; the extent of conversion, α:

$$\frac{d\alpha}{dt} = k(T)f(\alpha)$$

The temperature dependence of the process rate is typically parameterized through the Arrhenius equation:

$$k(T) = A \cdot exp\left(\frac{-E}{RT}\right)$$

The resulting equation provides a basis for differential kinetic methods.

$$\frac{d\alpha}{dt} = A \cdot exp\left(\frac{-E}{RT}\right) f(\alpha)$$

The governing equation is the 1D transient heat conduction:

$$\rho c_p \frac{\partial T}{\partial t} = \frac{\partial}{\partial x}\left(k \frac{\partial T}{\partial x}\right) + \dot{q}'''$$

Radiation enters through the boundary condition at $x = 0$. The net heat flux applied to the surface combines convection and radiation:

$$-k \left.\frac{\partial T}{\partial x}\right|_{x=0} = h(T_g - T_h) + \varepsilon(\dot{q}''_{inc} - \sigma T_w^4)$$

In-depth radiation absorption via the Beer-Lamber law:

$$\dot{q}'''_{rad}(x) = \kappa \dot{q}''_{inc} e^{-\kappa x}$$

10-dimensional parameter identification vector per decomposition reaction plus 5-dimensional vector for the char:

$$x = \left(A, E_a, n_s, \rho_0, c_p, k, \varepsilon, \chi, \Delta H_r, v_{char} \,|\rho^c, c_p^c, k^c, \varepsilon^c, \chi^c\right)^T \epsilon \mathbb{R}^{15}$$

SCE Global Optimization Algorithm

Inverse problem — minimize the MSE objective:

$$F(x) = \frac{1}{N}\sqrt{\sum_i \left(MLR_{sim}(t_i, x) - MLR_{exp}(t_i)\right)^2} \qquad x^* = \arg min\left(F(x)\right), x \in \Omega \subset \mathbb{R}^{15}$$

Population: s = p·m samples partitioned into p complexes of m points. Triangular selection weights for competitive complex evolution (CCE) sub-complex sampling:

$$p_i = {}^{2(m+1-i)}\!\Big/_{m(m+1)}, i = 1, \dots, m$$

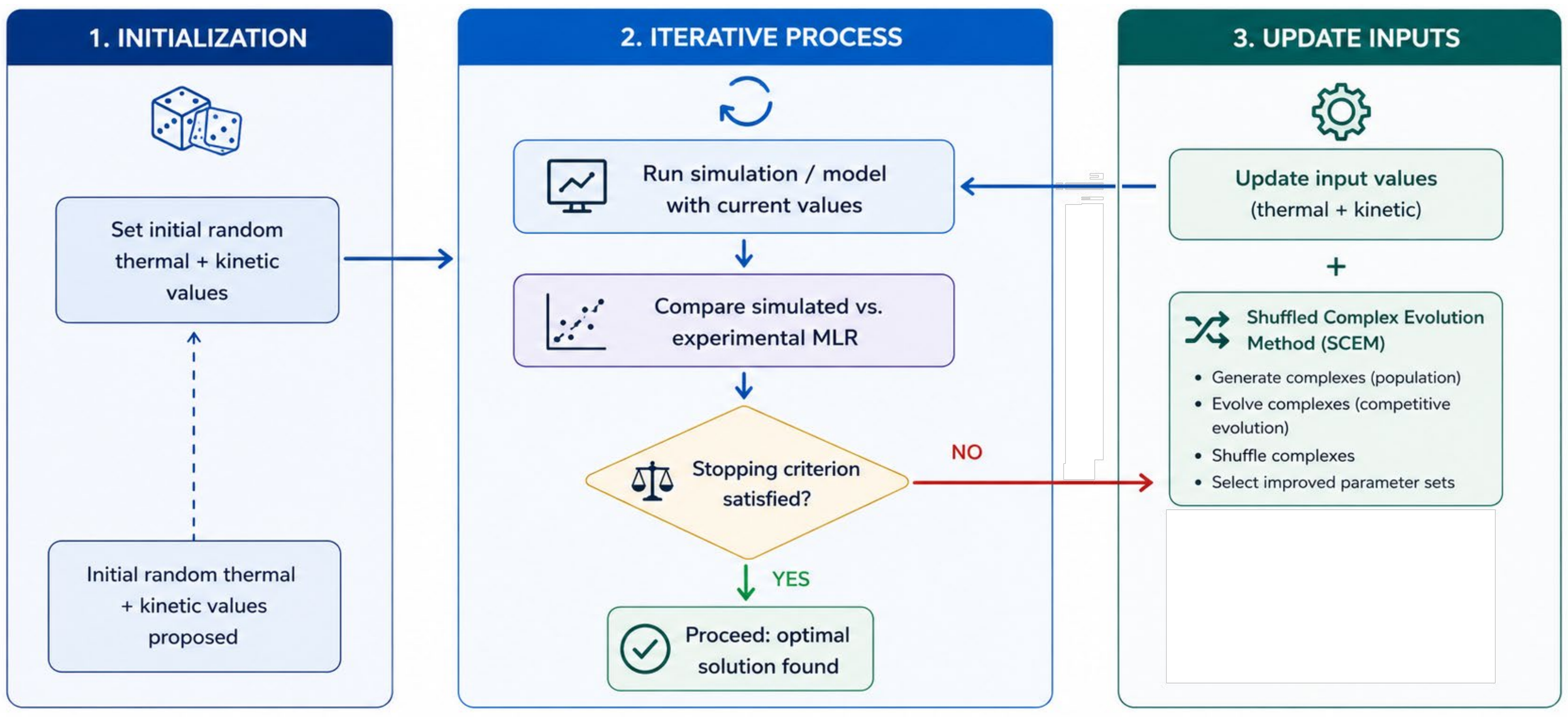
Select *q* different points $u_1, \dots, u_q$. CCE geometric operations (centroid, reflection, contraction):

$$g = [1/(q-1)] \sum_{j=1}^{q-1} u_j \qquad \textit{(centroid of q−1 best points)}$$

$$r = 2g - u_{worst} \qquad \textit{(reflection)}$$

$$c = (g + u_{worst})/2 \qquad \textit{(contraction)}$$

New point replaces worst point. Complexes are reshuffled after each CCE cycle; algorithm converges when Δx < tol or ΔF < tol.



1. INITIALIZATION

Set initial random thermal + kinetic values

Initial random thermal + kinetic values proposed

2. ITERATIVE PROCESS

Run simulation / model with current values

Compare simulated vs. experimental MLR

Stopping criterion satisfied?

NO

YES

Proceed: optimal solution found

3. UPDATE INPUTS

Update input values (thermal + kinetic)

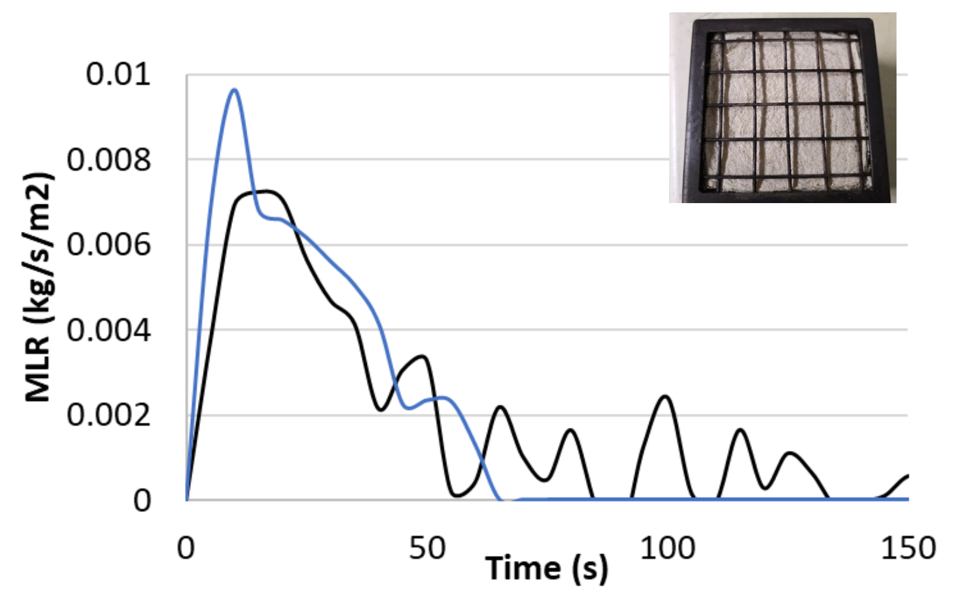
+

Shuffled Complex Evolution Method (SCEM)
- Generate complexes (population)
- Evolve complexes (competitive evolution)
- Shuffle complexes
- Select improved parameter sets

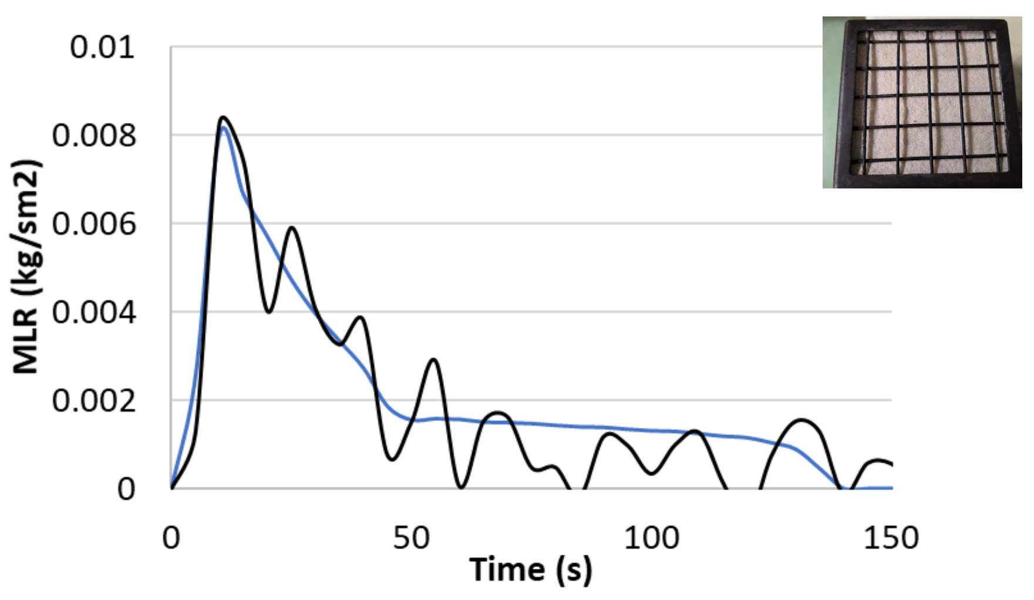
RESULTS & DISCUSSION

Calibrated simulations vs. experimental MLR data (cone calorimeter, ISO 5660-1, external heat flux 50 kW/m²).
Blue and black lines represent simulated and experimental results respectively.

Flax foam MLR comparison



Banana foam MLR comparison



Discussion

- Good agreement between simulations and experimental MLR for both materials
- SCE converges reliably in the 15-dimensional non-convex parameter space
- Banana-fibre foam slighly higher peak MLR than flax
- Identified Arrhenius parameters (A, E_a) are consistent with literature values for cellulosic bio-based materials

CONCLUSIONS

- SCE successfully identifies all 15 thermokinetic parameters for natural insulation foams from cone calorimeter data
- Calibrated model reproduces experimental MLR with high fidelity for both banana-fibre and flax-fibre specimens

FUTURE WORK / NOMENCLATURE

Future work:
- Extend to multi-step pyrolysis schemes
- Include analysis and validation with more types of materials

Nomenclature:

https://sciforum.net/event/iocma2026