Molecular Dynamics-based Resilience Assessment of Structures

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MIT CONCRETE SUSTAINABILITY HUB

More Than Elemental

According to the National Fire Protection Association (NFPA), losses due to fire in structures in America amount to around $13 billion annually. Despite these severe economic consequences, building codes often don't adequately predict the failure of an entire structure. Instead, they tend to model fire damage in individual elements without considering the greater building ensemble (all the elements together with their connections). Therefore, CSHub has developed a model that quantifies the complexity of fire at the element-scale (such as the spalling of concrete elements) as well as at the system-scale (accounting for any building use, geometry, etc.).

Figure 1: Fire induced spalling damage in the tunnel lining of the Channel Tunnel between England and France.

An Elegant Ensemble

Inspired by the molecular complexity of materials, our model simulates a building as an ensemble of atoms (elements) held together by bonds similar to those in molecules. This framework, known as a molecular dynamics modeling (MD), is attractive in comparison to traditional engineering methods due to its speed and ease of damage prediction. We use this model to predict charring on wood and spalling in concrete.

Spalling (**Figure 1**) is a form of fire damage that can occur when concrete's outer layers expand as they are heated while its colder core remains intact. Since spalling typically arises in concrete at around 400°C, we model it by removing any layer that reaches that temperature.

However, fire can lead to structural impacts besides spalling: For a complete model, we also accounted for concrete's strength and stiffness loss due to temperature. We then applied our approach to wood structures to facilitate a comparison with concrete.

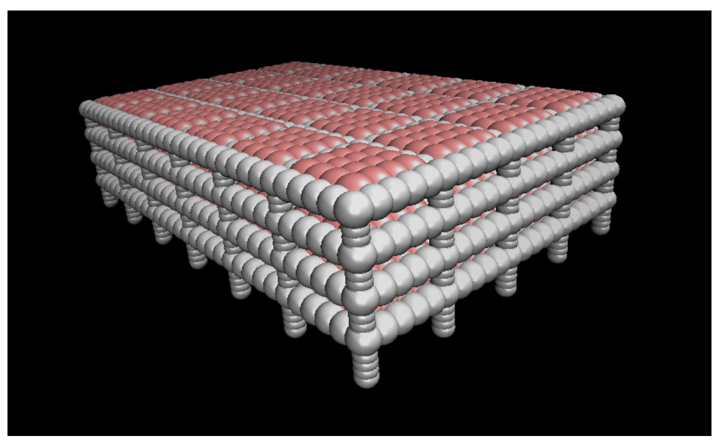

Figure 2: A typical layout of a Molecular Dynamics Model for the case of a DOE Reference Office Building (white masses represent column and beam elements while red masses represent slabs).

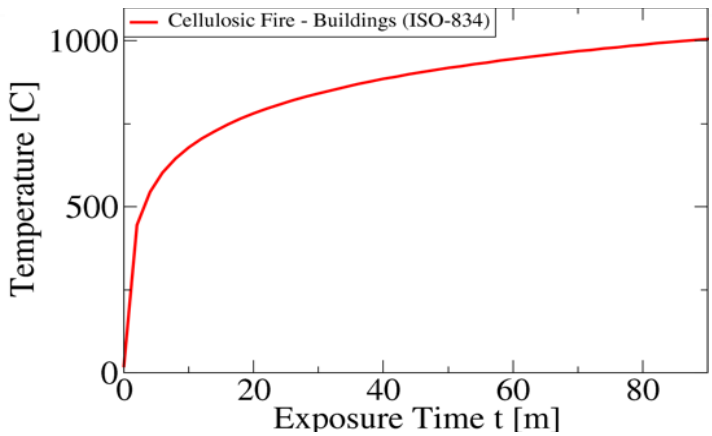

Figure 3a: Cellulosic Fire Curve

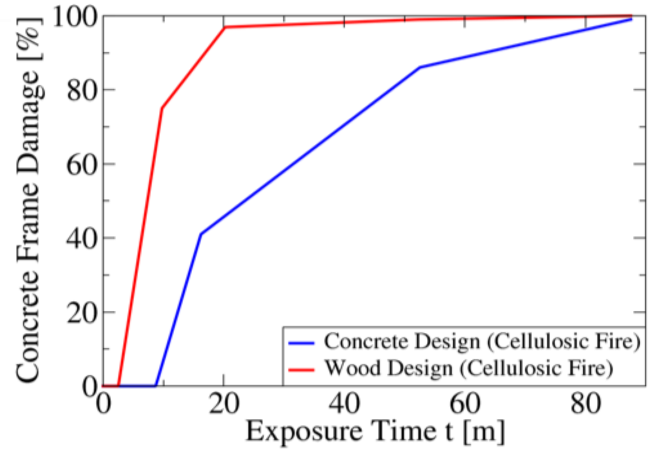

Figure 3b: Fragility Curves for Concrete and Wood Designs

Reevaluating the Risks

We modeled two different design solutions for the case study of a Department of Energy reference building (**Figure 2**) subjected to a standard building fire (cellulosic fire) (**Figure 3a**): a reinforced concrete design and a design where wood beams are connected to concrete columns through steel connections.

In **Figure 3b**, we show the fragility curves of these designs. While the wooden design fails at around 20 minutes due to rapid connection loss and wooden beam charring, the reinforced concrete frame fails at around 80 minutes from buckling due to the spalling of columns.

However, in IBC design codes, which consider elements separately, wood and concrete designs both have fire-resistance ratings of 90 minutes. This discrepancy suggests that design code standards may need reevaluation to account for all these complex phenomena at both the building- and element-scale.

Key Findings:

- The approach has significant advantages over traditional methods such as Finite Elements: absence of instabilities, ease of inelastic implementations, and speed of calculations.
- The model can easily simulate spalling, charring, and connection deterioration in real structures.
- System-scale fragility curves derived from the model can predict a structure's likelihood of failure.
- Our findings suggest that design codes may not consider all of the complex interactions that result from fire, especially those at the system-scale. Codes, then, should be re-evaluated based on this system-scale approach.

Related Links:

- CSHub Resilience Research
- Research Brief: Generating Building-specific Fragility Curves

Citation:

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