Coupled Multiphysics Simulation of Low-Temperature Belite Cement Formation via Combustion Synthesis

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THE WORLD'S GATHERING PLACE FOR ADVANCING CONCRETE

aci CONCRETE CONVENTION

Presentation outline

1. Need for novel manufacturing processes in the cement industry

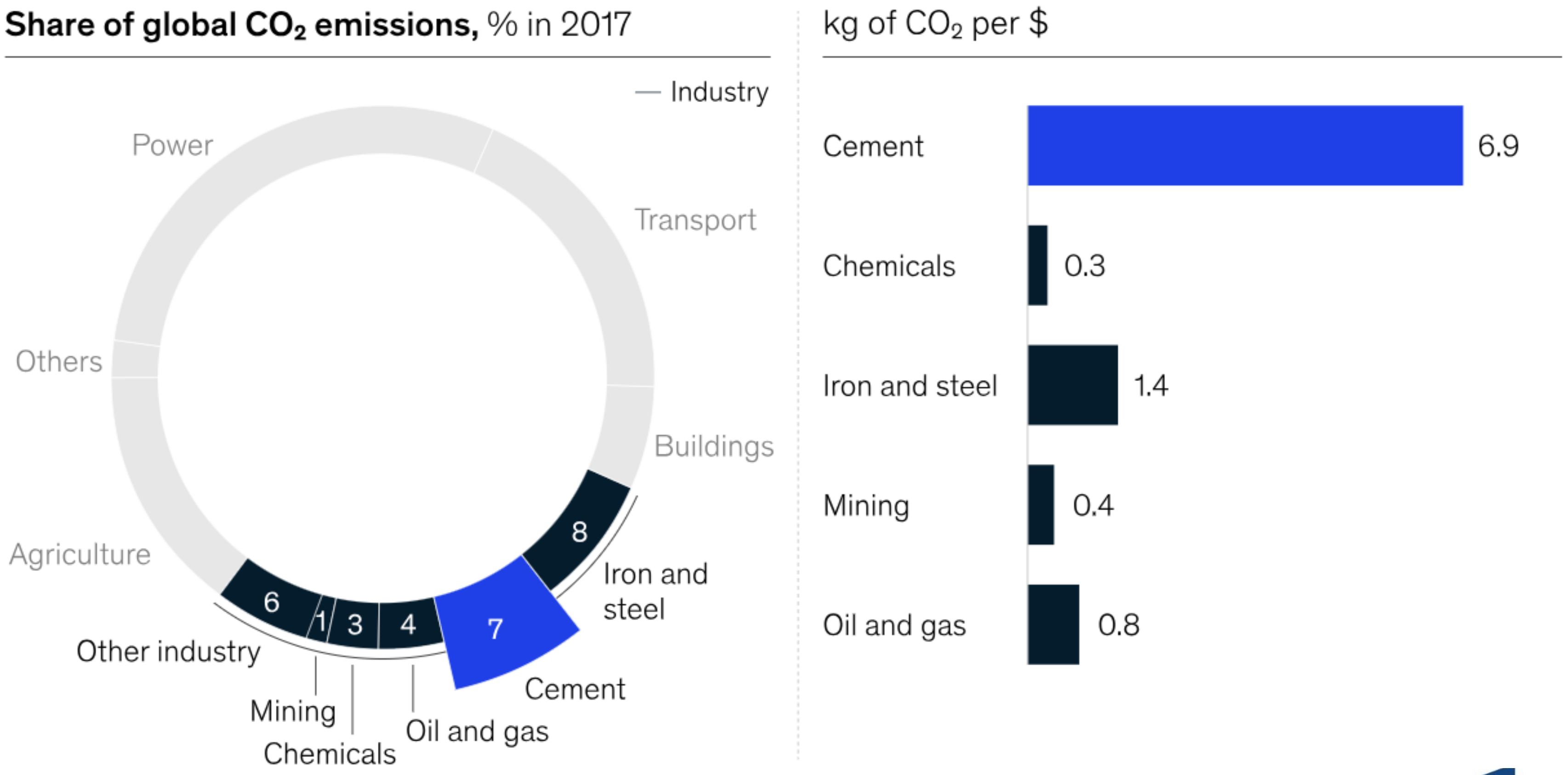
2. Introduction to biofuel-based combustion synthesis (BCS)

3. Numerical modeling of BCS pellets using COMSOL Multiphysics

4. Preliminary results and future work

1. Current State of the Cement Industry

Cement manufacturing is a major source of global CO_2 emissions and also generates the most emissions per revenue dollar.



Sector wise global CO_2 emissions and emissions per revenue dollar. (McKinsey, 2020)

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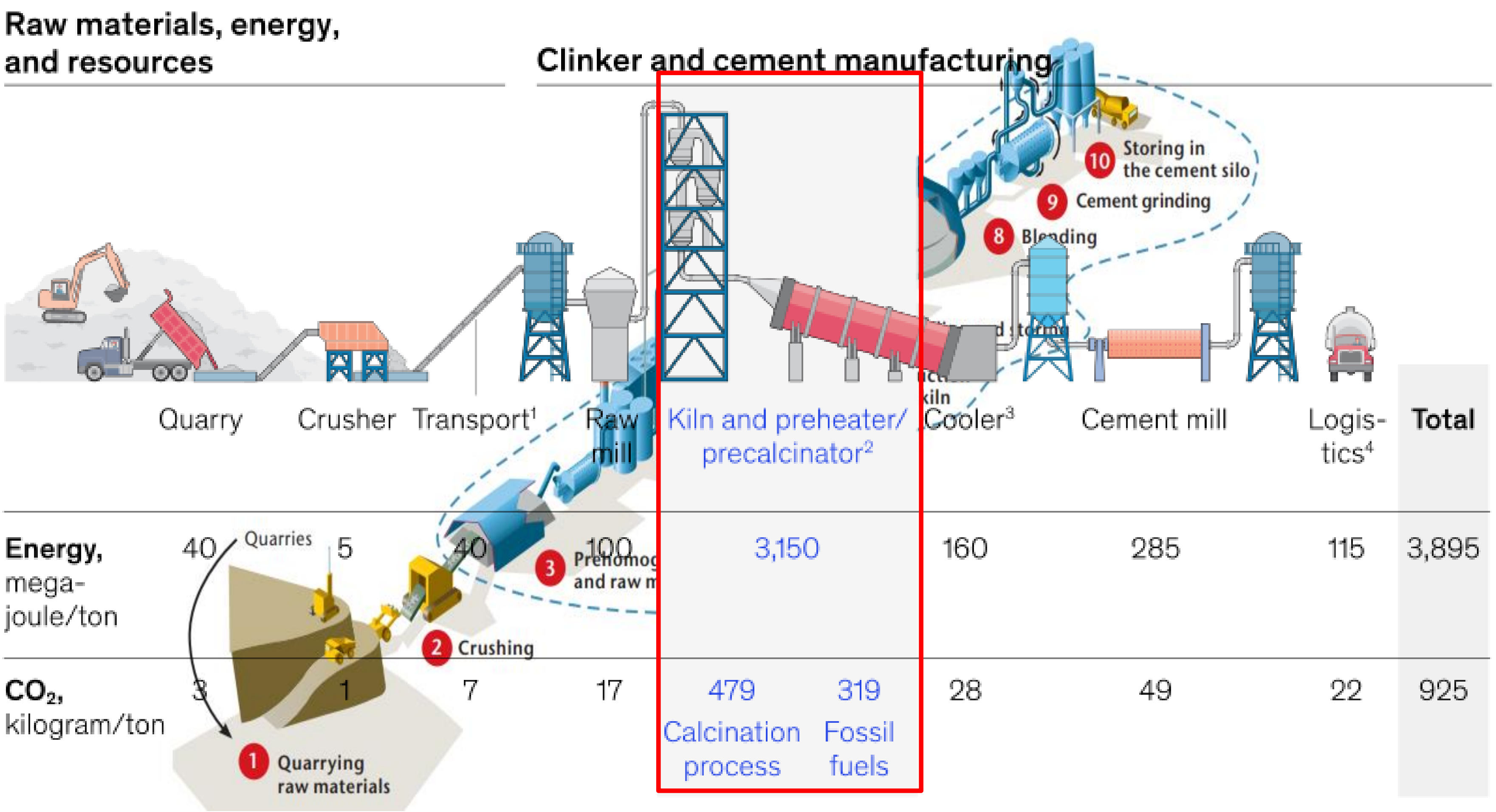
1. Current State of the Cement Industry

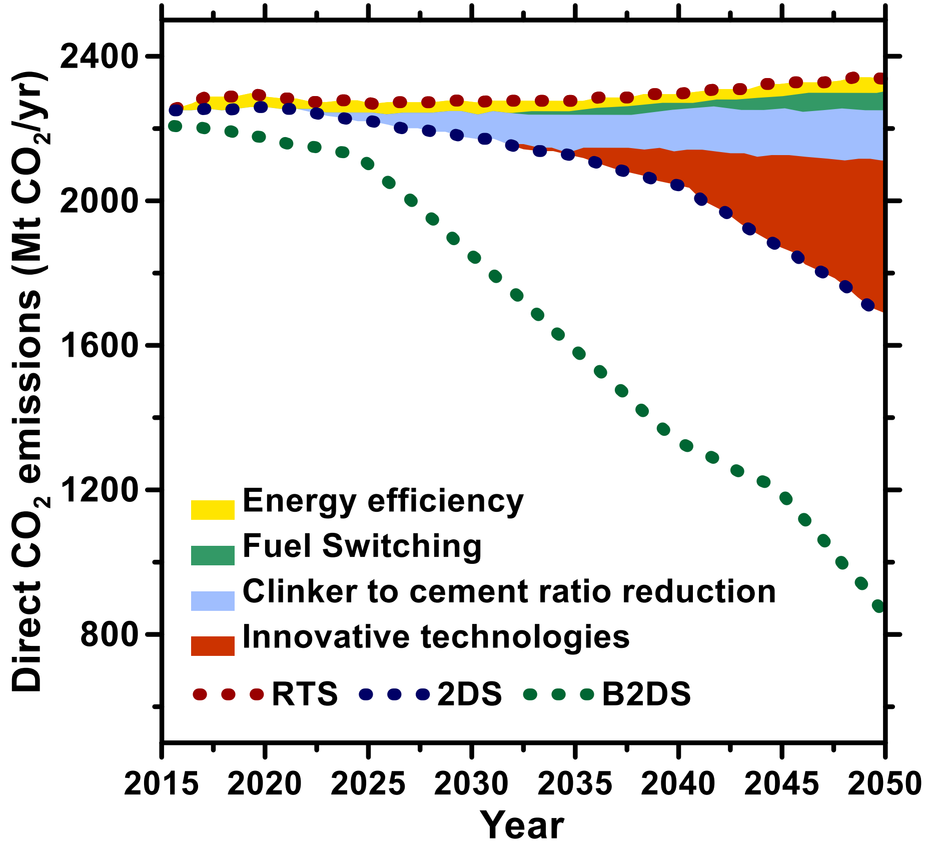


	Quarry	Crusher	Transport[1]	Raw mill	Kiln and preheater/ precalcinator[2]		Cooler[3]	Cement mill	Logis-tics[4]	Total
Energy, mega-joule/ton	40	5	40	100	3,150		160	285	115	3,895
CO_2, kilogram/ton	3	1	7	17	479 Calcination process	319 Fossil fuels	28	49	22	925

Conventional cement manufacturing process (IEA, 2015)

Emissions and energy breakdown in cement manufacturing steps (McKinsey, 2020)

1. Need for Novel Manufacturing Processes



Decarbonization pathway set out in IEA roadmaps (Volaity et al., 2025)

The projected cement demand is only increasing globally!

Urgent need to shift to better manufacturing processes.

Novel manufacturing method targeting the levers mentioned in IEA roadmaps: Biofuel-based Combustion Synthesis (BCS)

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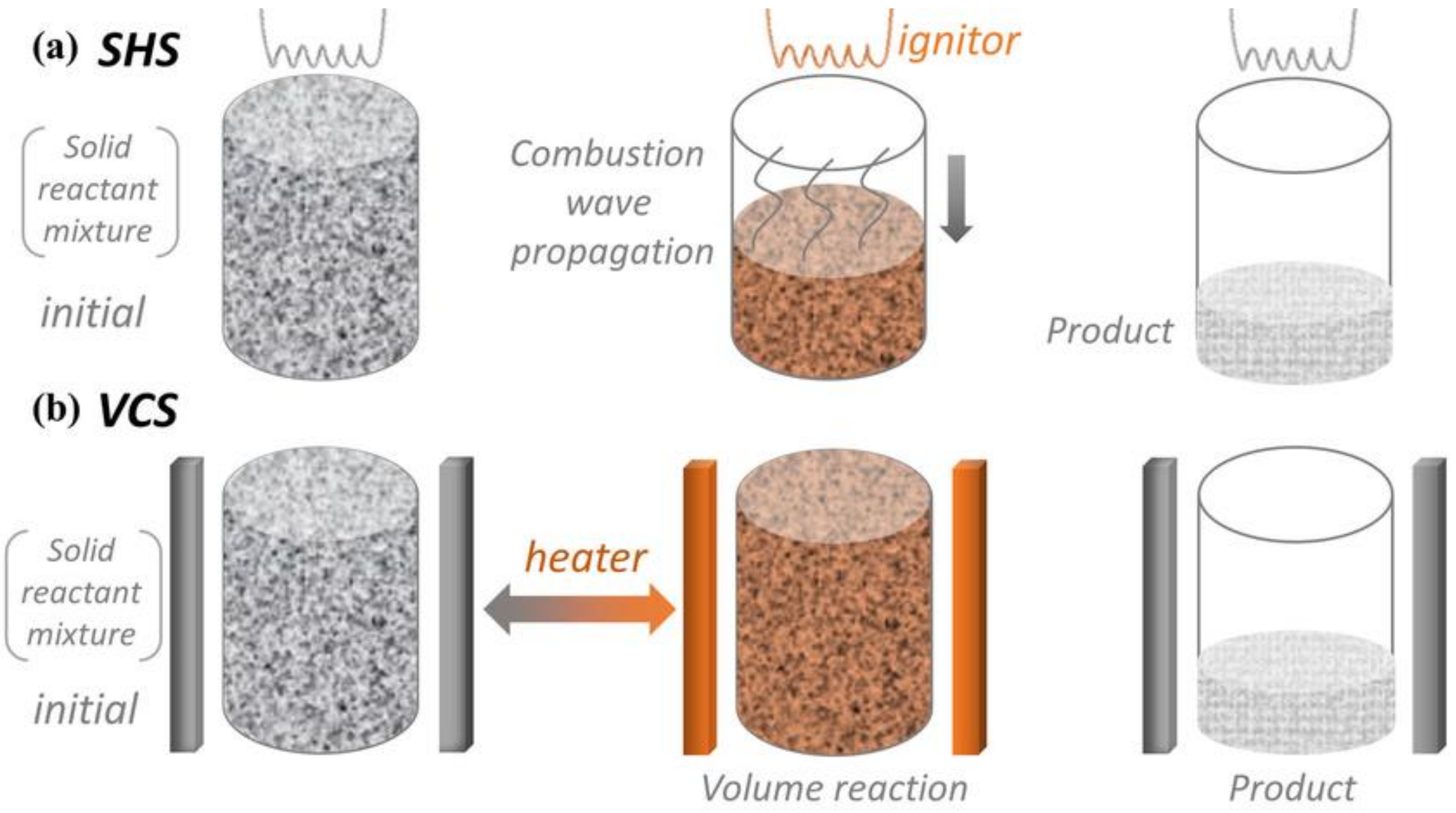
2. Biofuel-based Combustion Synthesis

- Combustion synthesis (CS), also Self-propagating High-temperature Synthesis (SHS)
- **CS/SHS: Utilizes heat from an exothermic combustion reaction to initiate a synthesis reaction.**
- Use of biofuel for combustion: Biofuel-based Combustion Synthesis (BCS)



Schematic representation of SHS and volumetric combustion synthesis (VCS) (Carlos et al., 2020)

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2. BCS and Decarbonization Pathways

BCS enables low-temperature synthesis of cement and its precursors

- **Limestone calcination** at **450 °C as opposed to ~800-900 °C** conventionally
- **Belite cement synthesis** at **700 °C as opposed to ~1200-1300 °C** conventionally

→ **Improving energy efficiency**

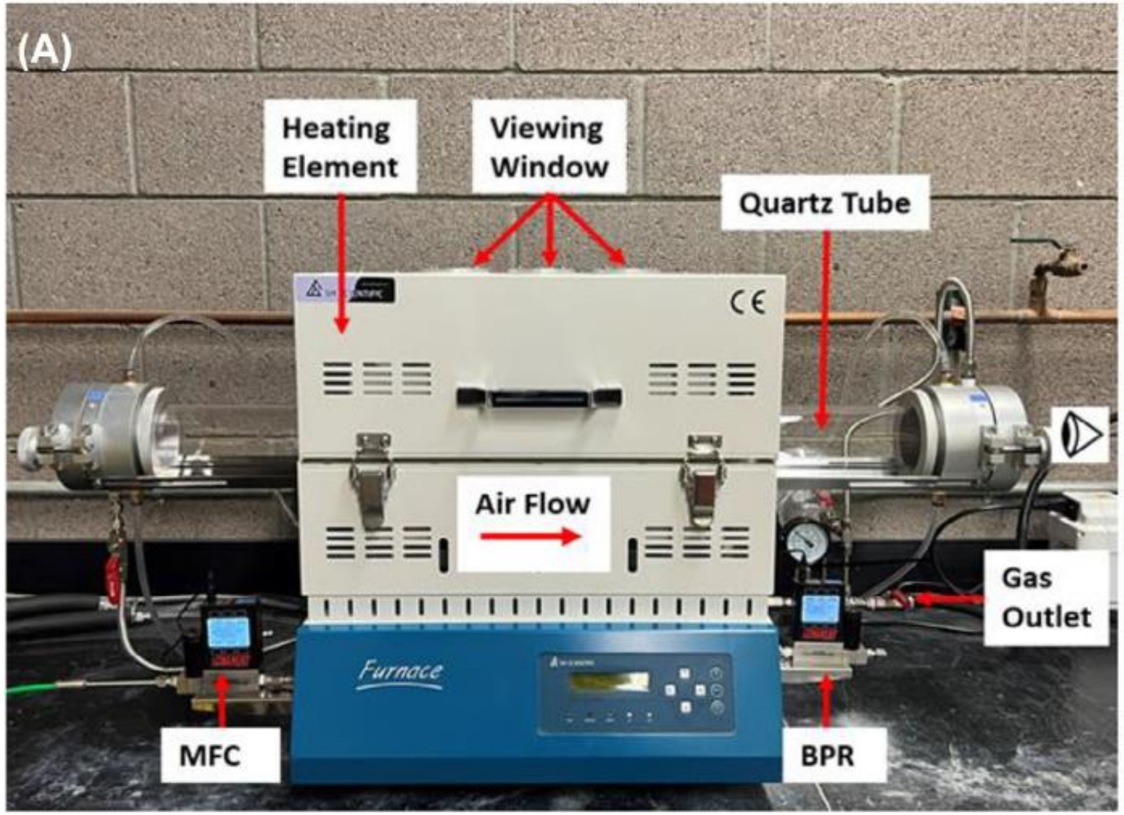
2. BCS and Decarbonization Pathways

Use of **biofuels such as lignin and biomass** instead of conventionally used coal and petroleum products. → **Fuel Switching**

Synthesis and use of **belite cement** instead of OPC. → **Innovative Technologies**

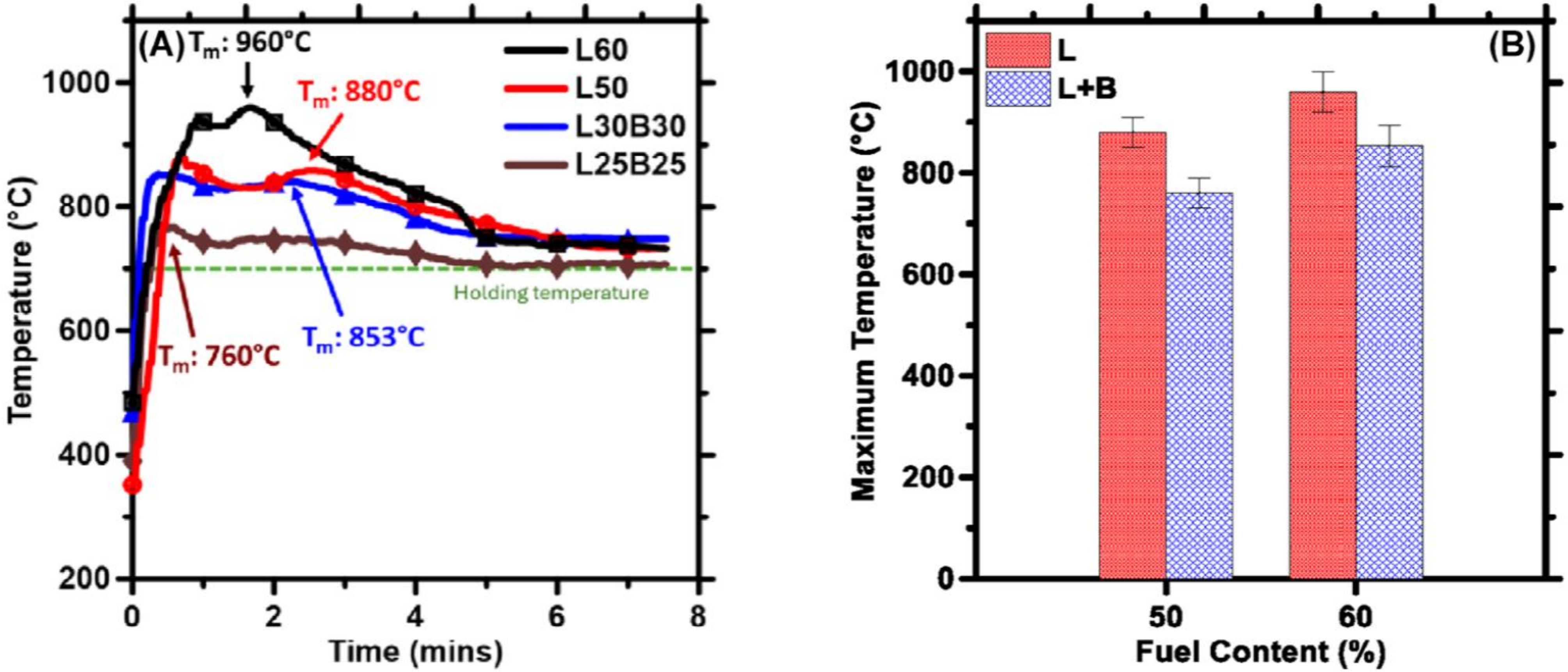
2. BCS Experimental Setup

1. 2.5 grams of raw materials proportioned.
2. Limestone & silica at 3:1 ratio + biofuel mixed and pelletized (R:12.7mm H:15mm).
3. Initial treatment in oven at 50 °C for 12 hrs. to remove water.
4. Pellet introduced to furnace set at 700 °C.
5. Air flow enabled to assist combustion.
6. Surface temperature measured using infrared camera.
7. Biofuel combustion enables belite formation.



BCS experimental setup (Agrawal et al., 2025)

2. BCS Experiment Results



L – lignin

B – biomass

L60 – pellet with 60% lignin content.

(a) Surface temperature evolution; and (b) Maximum surface temperature for different pellet cases
(Agrawal et al., 2025)

2. BCS Experiment Results

Maximum surface temperature and belite content by mass for different pellet cases (Agrawal et al., 2025)

Fuel type/content	Holding time (min)	Holding temperature (°C)	Max. surface temperature (°C)	C_2S content (% by mass)
L50	15	700	**880 ± 20**	**78 ± 2**
L25B25	15	700	**730 ± 30**	**76 ± 4**
L60	15	700	**983 ± 30**	**83 ± 4**
L30B30	15	700	**800 ± 50**	**80 ± 2**

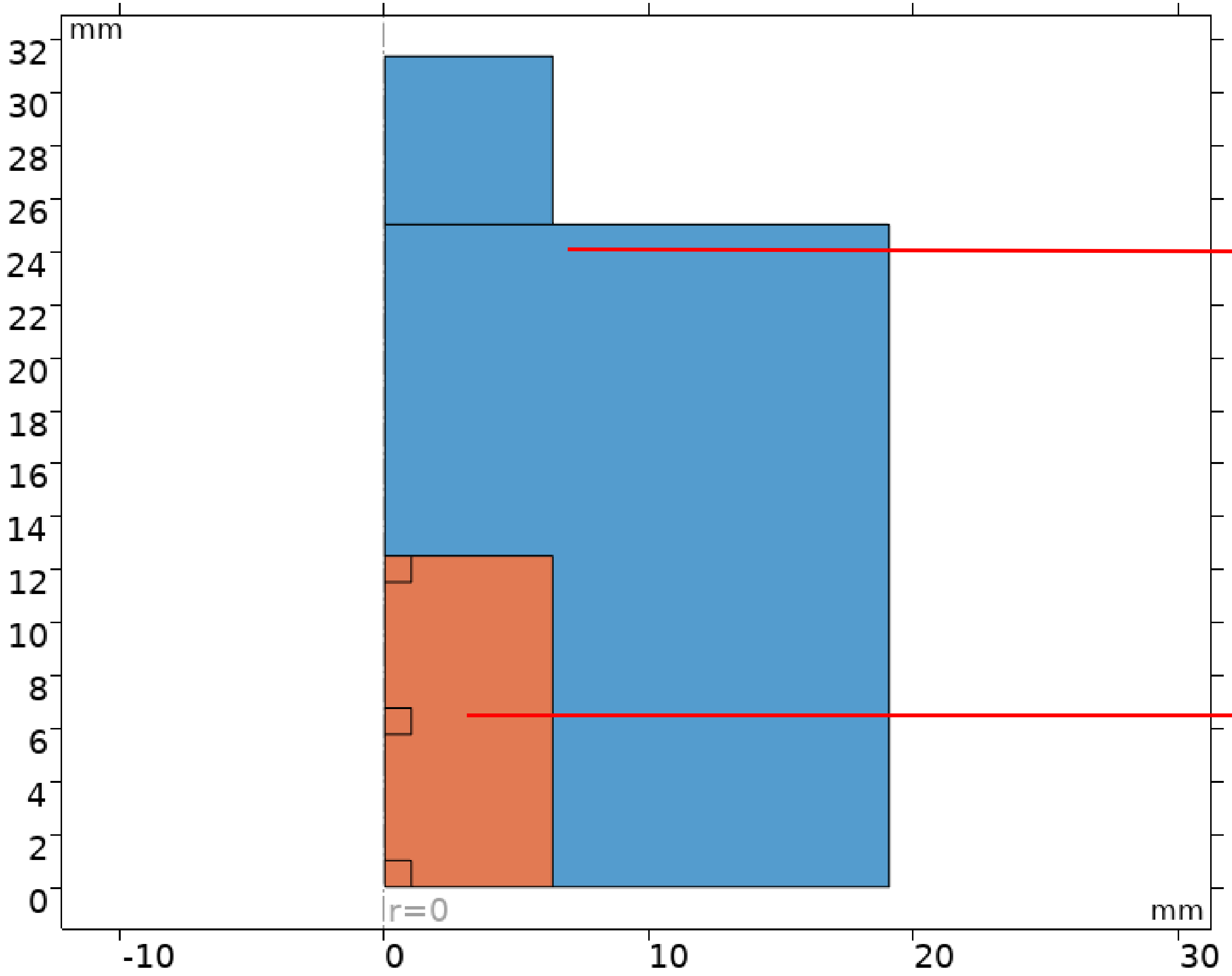
L – lignin
B – biomass
L60 – pellet with 60% lignin content.

3. Need for Numerical Simulations

- **Experiments only reveal the surface temperature.**

  Internal temperatures can be higher → high temperature applications (OPC)
- To accelerate **process optimization.**
- To provide mechanistic insights into the process
  - Experiments can give outcomes → simulations can **explain why those outcome happen.**
  - Track feedback loops, how one experimental factor alters the effect of another factor, etc.
- Advancement over prior SHS/CS modeling in literature.

3. Multiphysics Model: Geometry



Furnace

- Air
- @ 700 °C

Porous pellet

- Raw materials + pore space
- @ 50 °C
- 8% porosity as determined from experiments

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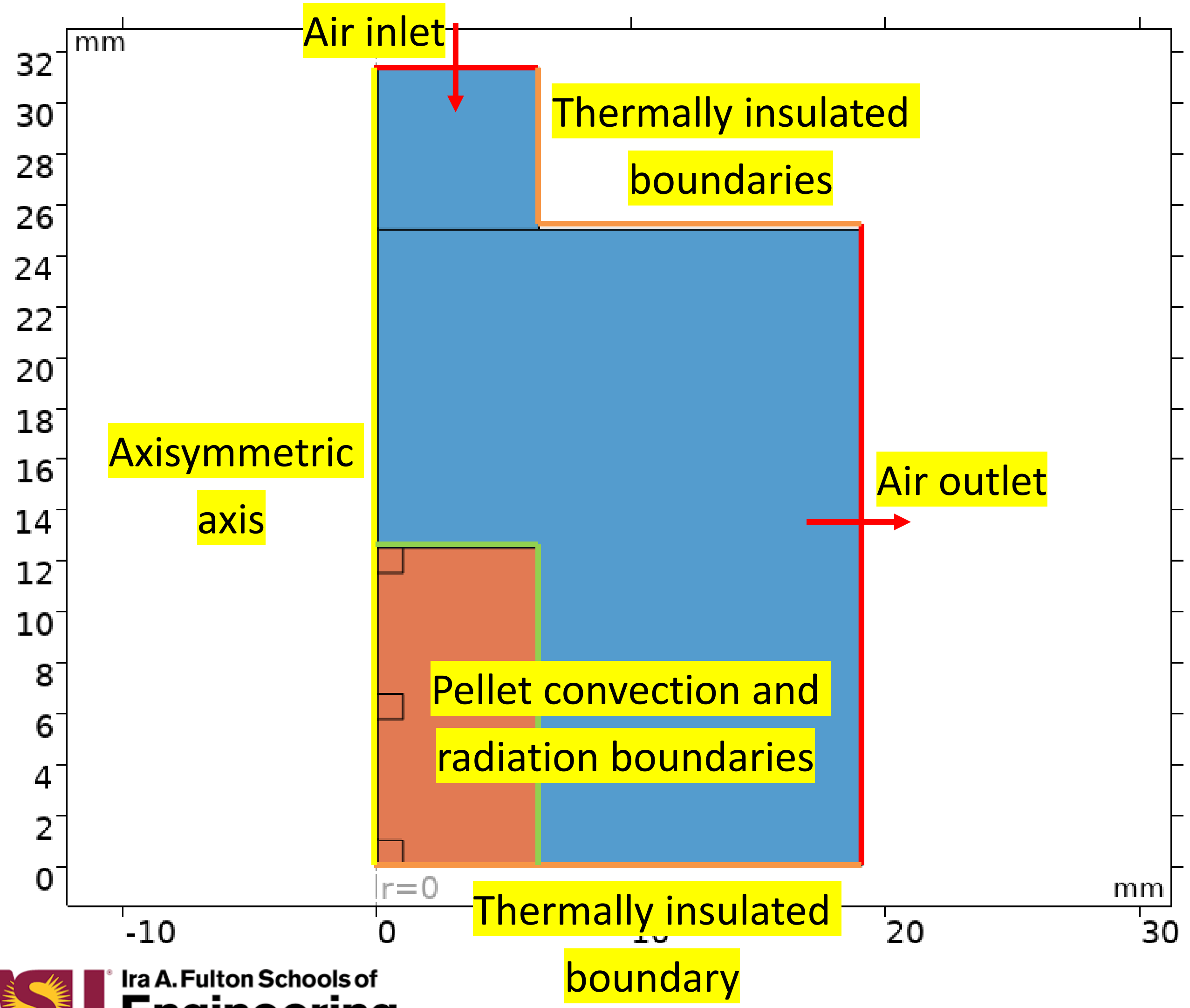
3. Multiphysics Model: Boundary Conditions



Physics accounted for

- Heat transfer
- Fluid flow
- Species transport
- Chemical reaction kinetics

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3. Multiphysics Model: Physics

Multiphysics Coupling

- Heat transfer equation used to solve for the temperature field.
- Fluid flow to solve for velocity and pressure fields
  - Navier-Stokes equation for the fluids in furnace domain.
  - Brinkman equations for the fluids in the pellet domain.
- Mass transport equation used to solve for the fluid species concentrations.
- Domain ODEs defined for reaction kinetics and solid species densities.

3. Multiphysics Model: Physics

Domain ODEs – Reaction Kinetics

α: degree of reaction
A: Pre-exponential factor
E: Activation energy

1. Biofuel combustion

$CH_{1.44}O_{0.66} + 1.03\ O_2 \rightarrow CO_2 + 0.72\ H_2O$

$$\frac{d\alpha_1}{dt} = A_1 e^{\frac{-E_1}{RT}}(1-\alpha_1)$$ First order

2. Limestone calcination

$CaCO_3 \xrightarrow{\Delta} CaO + CO_2$

$$\frac{d\alpha_2}{dt} = A_2 e^{\frac{-E_2}{RT}}\left[2(1-\alpha_2)^{\frac{1}{2}}\right]$$ Contracting geometry

3. Belite synthesis

$CaO + SiO_2 \xrightarrow{\Delta} 2CaO.(SiO_2)$

$$\frac{d\alpha_3}{dt} = A_3 e^{\frac{-E_3}{RT}}\left[\frac{3(1-\alpha_1)^{\frac{2}{3}}}{2\left(1-(1-\alpha_1)^{\frac{1}{3}}\right)}\right]$$ Diffusion controlled

3. Multiphysics Model: Physics

Model Inputs

1. Heat from reactions

$$Q_{tot} = \sum\left(-\Delta H_i \rho_{i,0} \frac{d\alpha_i}{dt}\right)$$

2. Species source due to reactions, CO_2 for example,

$$S_{w,CO_2} = \left(\frac{-1}{M_{w,CO_2}}\frac{d\rho_{LG}}{dt}\right) + \left(\frac{-1}{M_{w,CO_2}}\frac{d\rho_{LS}}{dt}\right)$$

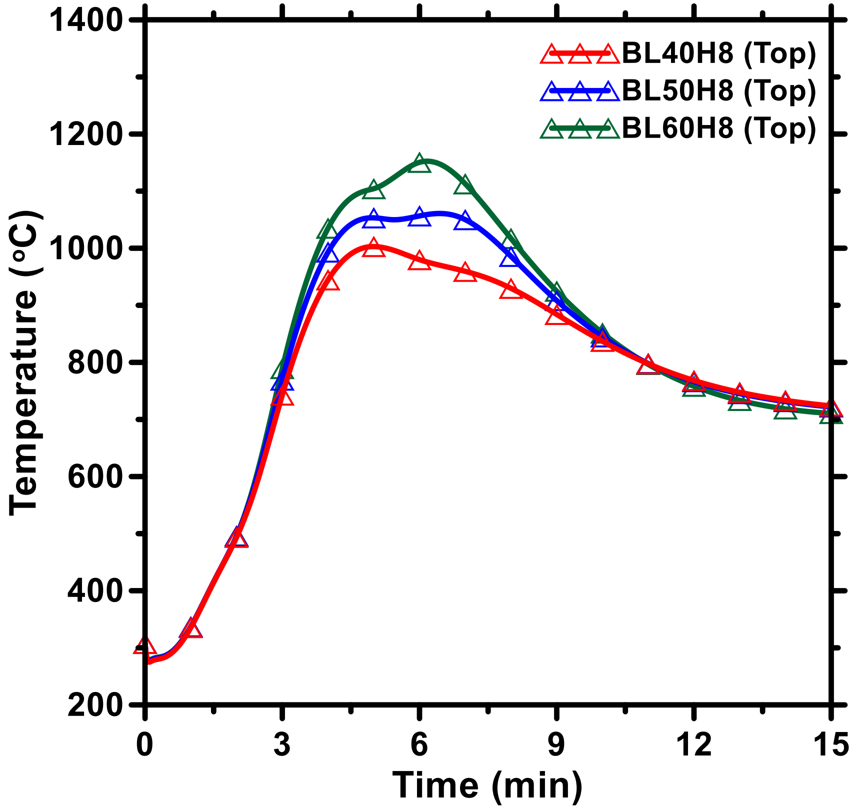
3. Porosity of the pellet,

$$\epsilon_p = 1 - \left(\frac{\rho_{LG}}{\rho_{LG,true}}\right) - \left(\frac{\rho_{LS}}{\rho_{LS,true}}\right) - \left(\frac{\rho_{LI}}{\rho_{LI,true}}\right) - \left(\frac{\rho_{SI}}{\rho_{SI,true}}\right) - \left(\frac{\rho_{C_2S}}{\rho_{C_2S,true}}\right)$$

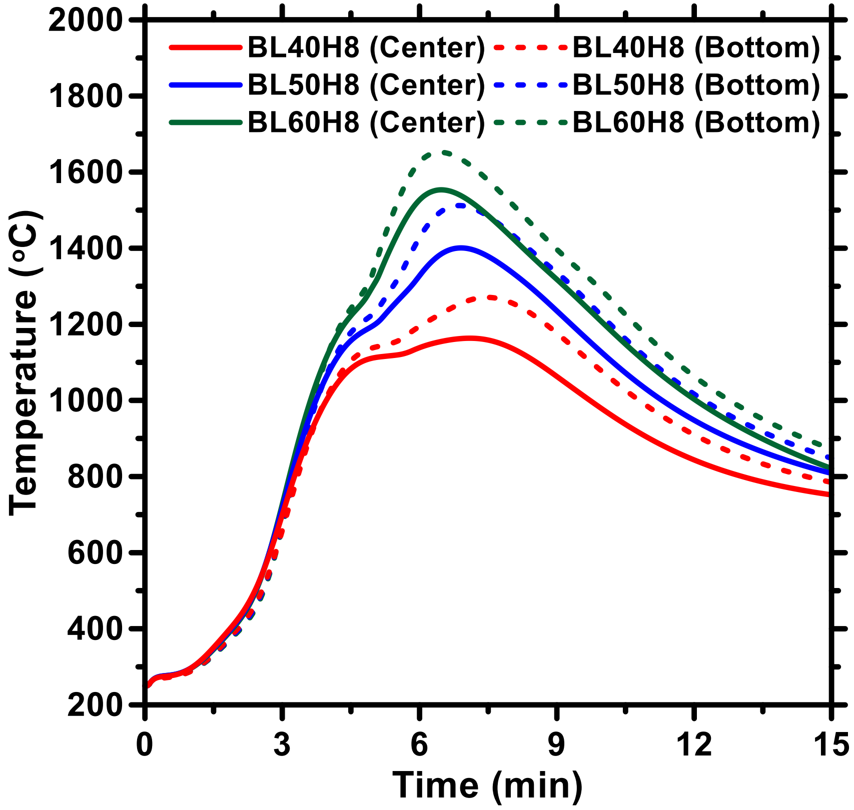
$\boldsymbol{\rho}$: density, $\boldsymbol{\Delta H}$: enthalpy of reaction, $\boldsymbol{M_{w,CO_2}}$: molecular weight, **LG:** lignin, **LS:** limestone, **LI:** lime, **SI:** silica

4. Preliminary Results

Temperature Profiles



Surface temperature evolution



Core temperature evolution

BL40H8

Belite pellet

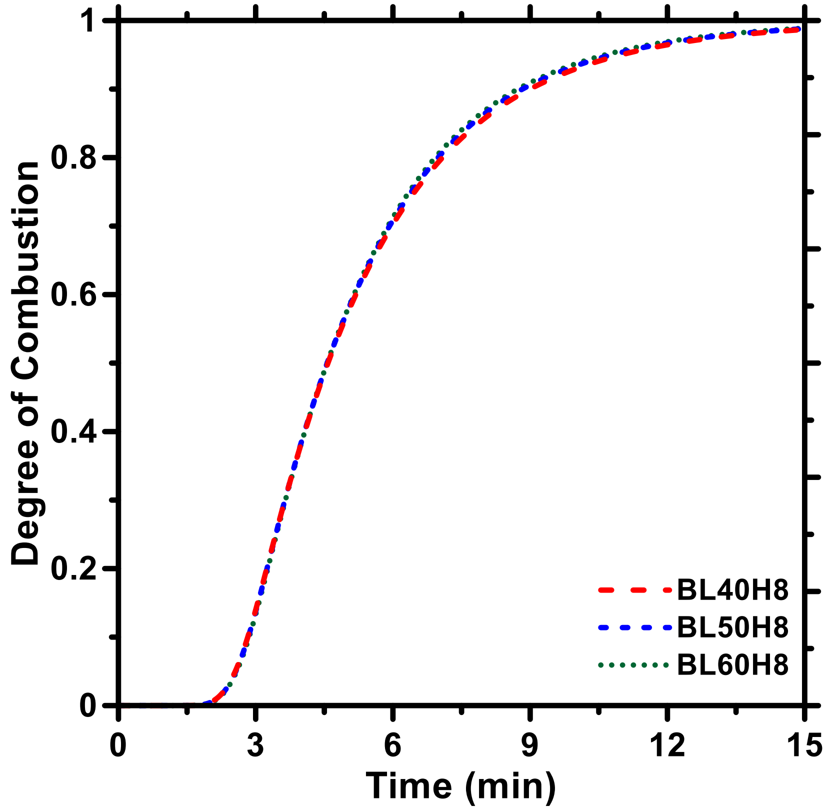
40% Lignin content

Half inch radius

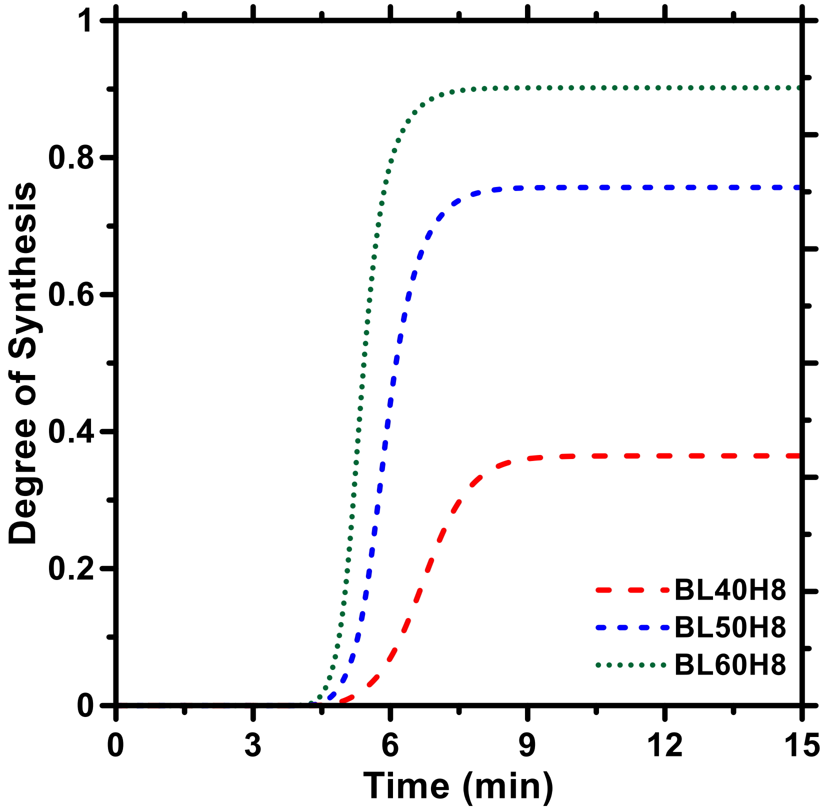
8% porosity

4. Preliminary Results

Degree of Reaction Progression



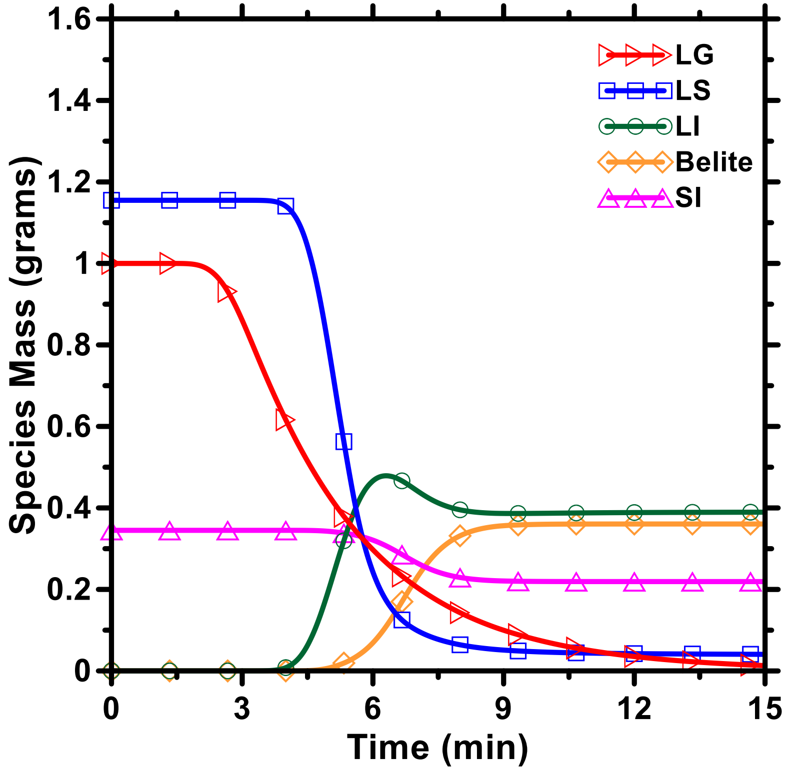
Fuel degree of combustion for different pellet cases



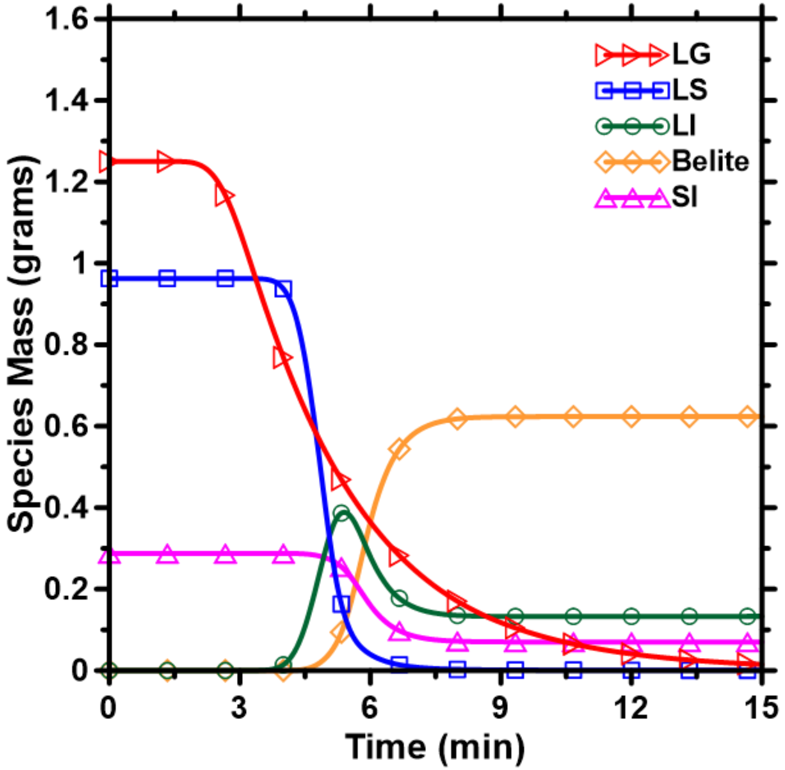
Belite degree of synthesis for different pellet cases

4. Preliminary Results

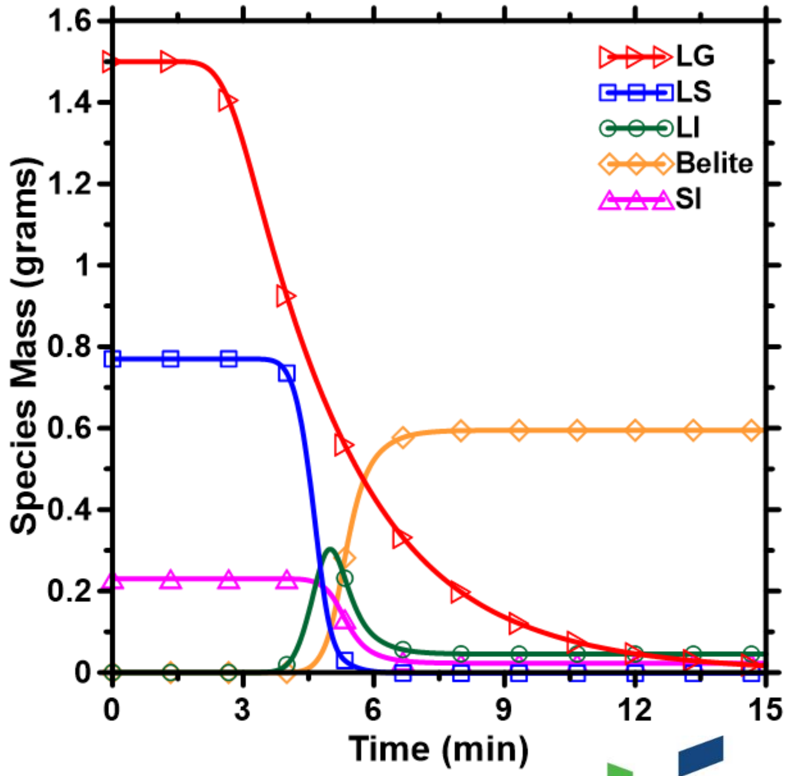
Solid Species Mass Evolution



Solid species mass evolution for ***BL40H8***



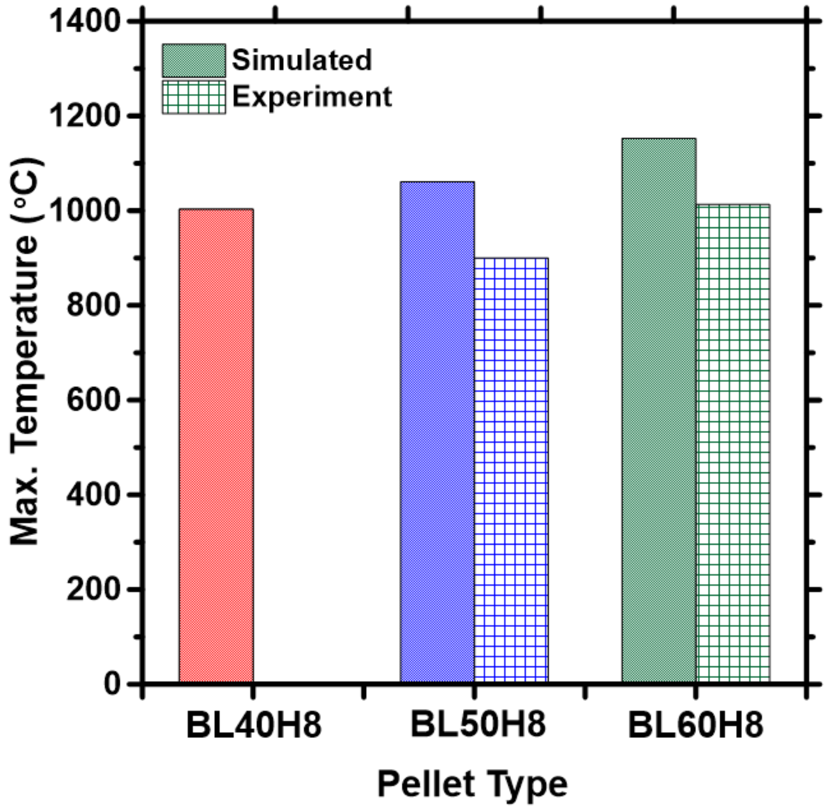
Solid species mass evolution for ***BL50H8***



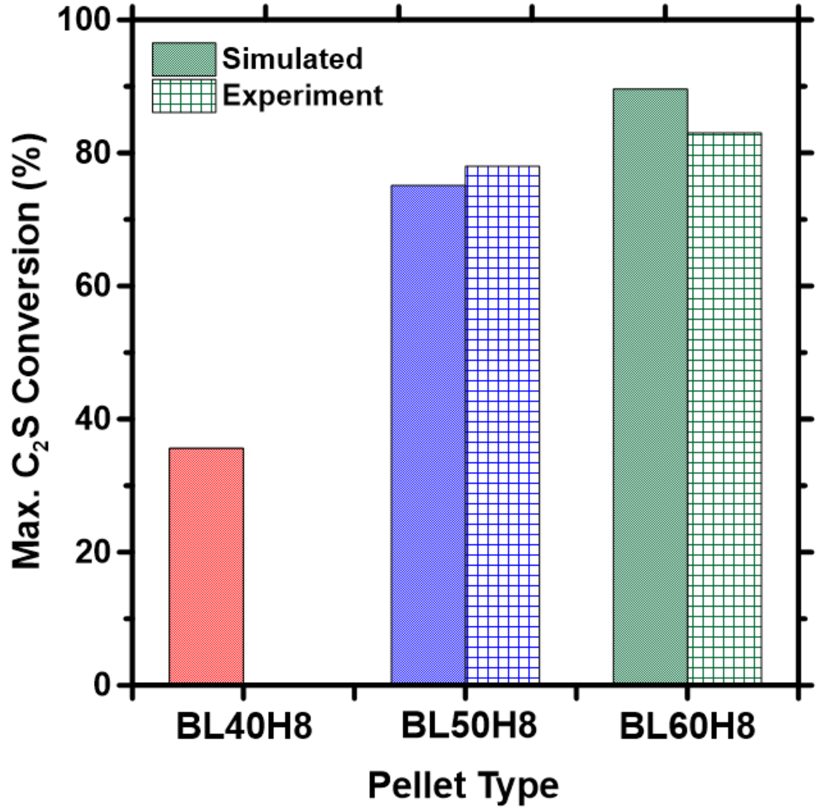
Solid species mass evolution for ***BL60H8***

4. Preliminary Results

Comparison with Experiments



Max. surface temperature of pellets simulation vs. experiments



Max. belite conversion percentage of pellets simulation vs. experiments

4. Conclusions and Future Work

- Preliminary results from simulations correlate well with experiments.

- Future work
  - Studying more pellet cases to reveal more mechanistic interpretations.
  - Characterizing the thermal wave propagation properties.
  - Extending the modeling framework for high-temperature applications such as OPC synthesis.

Thank you!

Questions and comments?

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