Development of Mathematical Model and Simulation For High Capacity Production of Carbon Fiber

HPC4Mfr CRADA No. NFE-17-06446

ORNL, Harper International

May 2017-Nov 2018

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U.S. DOE Advanced Manufacturing Office Program Review Meeting

Washington, D.C.

June 11, 2019

Overview

Project Title: Development of Mathematical Model and Simulation For High Capacity Production of Carbon Fiber

Timeline:

Project Start Date: 05/01/2017

Budget Period End Date: 11/30/2018

Project End Date: 11/30/2018

Project Budget and Costs:

Budget	DOE Share	Cost Share	Total	Cost Share %
Overall Budget	$300,000	$60,000	$360,000	20.0%
Approved Budget (BP-1&2)				
Costs as of 3/31/19				

Barriers and Challenges:

- Understanding the process of off-gas mixing with the nitrogen cover gas into purge gas which critically affects the fiber properties.
- Maintaining uniform temperature and atmosphere conditions across the width of the furnace in order to ensure uniformity of the resulting properties of carbon fiber.

Project Team and Roles:

Srdjan Simunovic (ORNL)-PI
Srikanth Allu (ORNL)-Technical Lead
Tae-Seok Lee (Harper International)-PI Industry

AMO MYPP Connection:

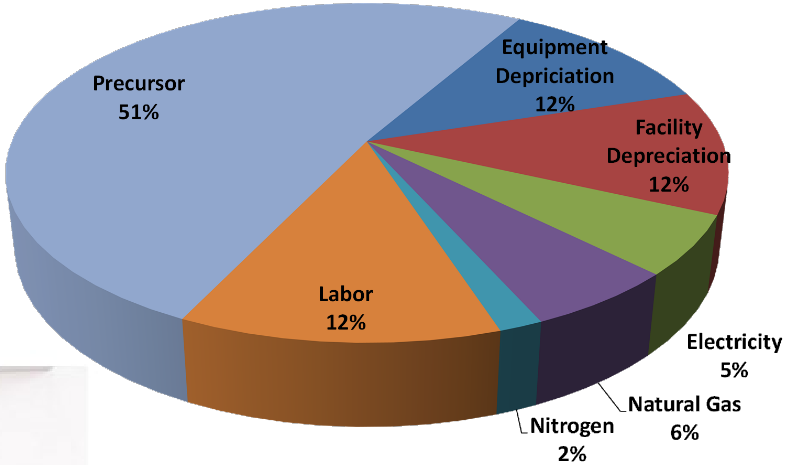
- Target 7.1: Reduce production cost of finished carbon fiber composite components for targeted clean energy applications by 50% compared to 2015 state-of-the-art technology.

- Target 7.3: Develop manufacturing technologies that reduce the embodied energy and production-associated greenhouse gas (GHG) emissions of carbon fiber reinforced polymer (CFRP) by 75% compared to 2015 typical technology.

Project Objective(s)

- Processing calculations show that the current ‘state of the art’ 1500TPY carbon fiber line uses 30kW of energy to produce 1 kg of fiber. A scaled up line capable of making 10,000TPY will need only about 12.5kW/kg, with more than 50% of energy savings with a commensurate savings in cost
- Increasing the production capacity and process efficiency of carbon fiber plants requires larger, faster and more energy efficient furnaces.
- The main technical challenges are:
  - Understanding the process of off-gas mixing with the nitrogen cover gas into purge gas which critically affects the fiber properties.
  - Maintaining uniform temperature and atmosphere conditions across the width of the furnace in order to ensure uniformity of the resulting properties of carbon fiber.

Carbon Fiber Market



Demand for low cost CFRP is increasing, especially in automotive industry.

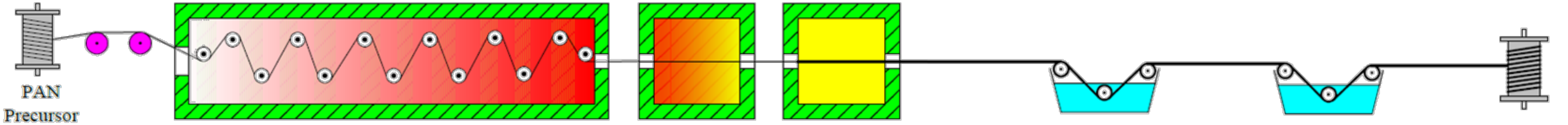
Cost of Manufacturing

1500 ton/year 12k tow

The passenger frame of BMW's i3 is fashioned from lightweight carbon fiber Courtesy Auto Motorund Sport, Germany

Carbon Fiber Low Temperature Furnace

The carbonization process converts stabilized precursor PAN fiber into carbon fiber inside LT furnaces.



Current state of art/Literature Review

- At system level tension and temperature play significant role for efficient carbonization of PAN fiber tows at large scale
- There is no modeling capability that could address all relevant physical phenomenon in processing carbon fiber at plant level
- Coupled plant scale conditions with fiber pyrolysis reaction mechanism that can predict chemical composition and properties of fiber will be an indispensable tool for carbon composites community

Project Approach

Develop parametric computational models for heat transfer, gas flows and fiber carbonization inside the carbon fiber furnace. The developed models are used to investigate various design strategies for scaling up carbon fiber furnaces.

The model integrates heating and kinetic thermochemical models of the fiber carbonization, and the three-dimensional computational fluid dynamic model of mixing of off-gases from carbonization and purge gas.

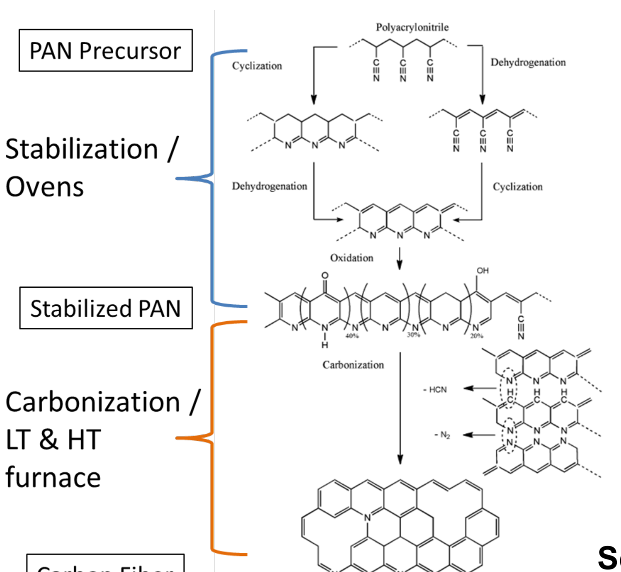
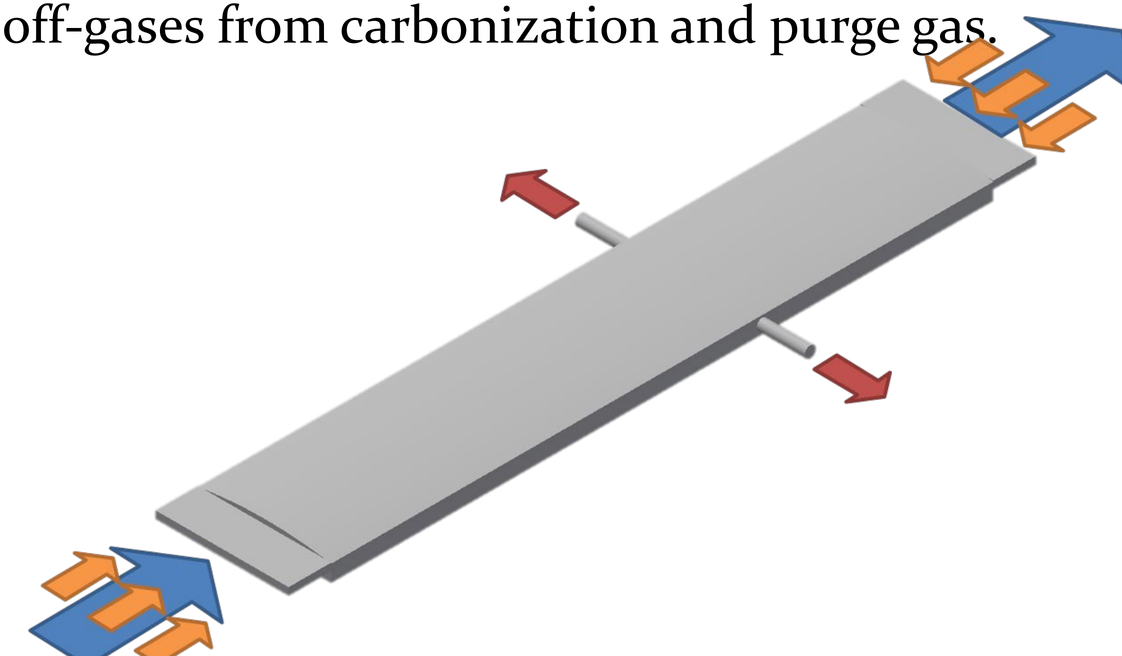


Figure 5. Model reaction paths from PAN to carbon phase.



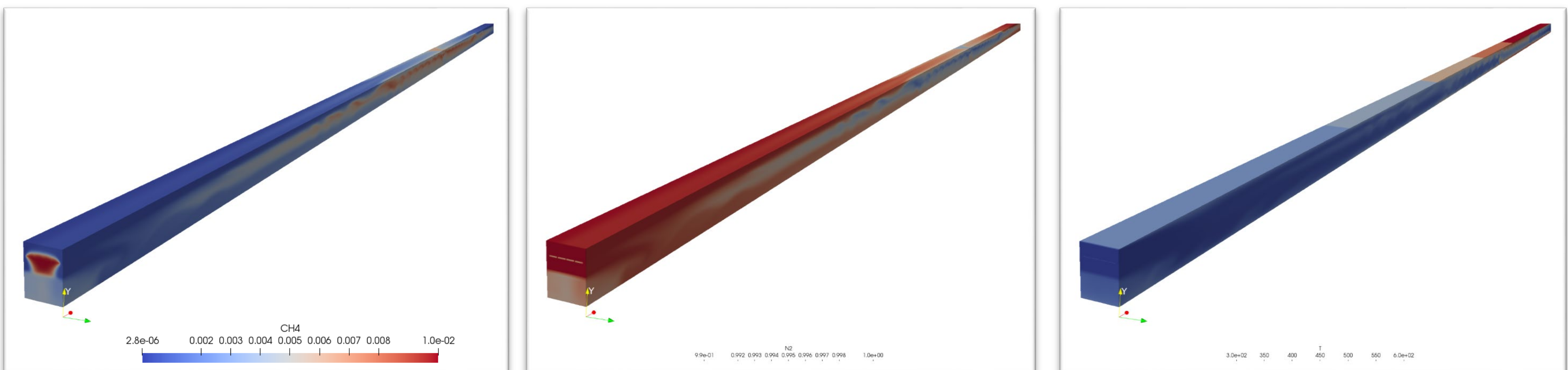
Schematic of the LT furnace model
Studied the CFTF LT furnace has 4 temperature compartments with transition regions in between.

Technical Approach

- Fiber region is modeled as multiple separated tow bands across the furnace width. This accounts for gas flow effects through the fiber region and fiber temperature variation in the furnace with direction.
- Fibers are heated by the radiation from furnace walls. Off-gas, a by-product of the fiber conversion process, mixes with the purge gas and interacts with the fiber region via convection. Full energy balance equations are solved in all furnace regions.
- Fiber conversion is modeled as a single step reaction with release of off gas into furnace chamber. Multi-step reactions can be added as needed.

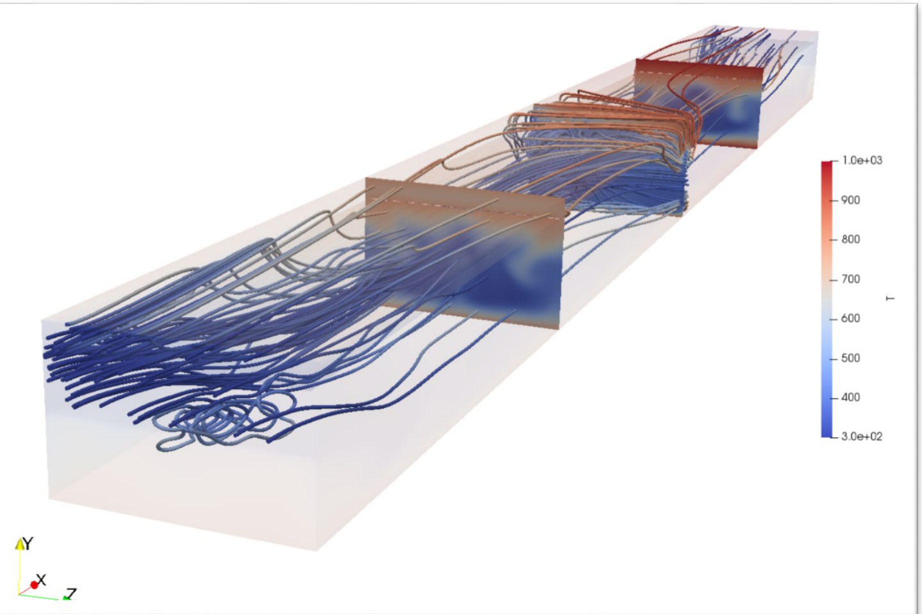
Results and Accomplishments

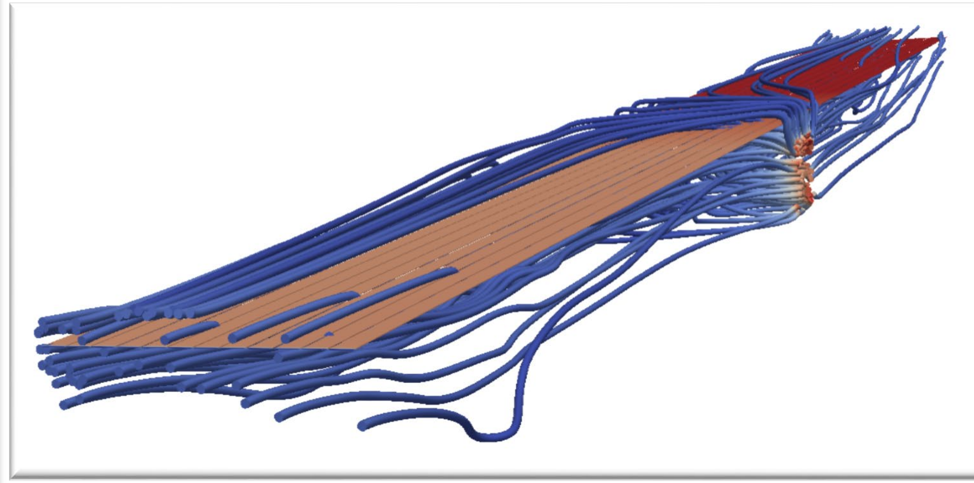
- The current model assumes two species, purge gas (N_2) and off-gas. We model off-gas as methane (CH_4). The two species gas flow are non-reacting. Harper Inc. has developed a single step reaction kinetics of species for off-gas that was included into the model.



Methane and nitrogen distribution in the furnace.

Results and Accomplishments





Left: Gas flow stream tracers color-coded with off-gas(CH_4) fraction distribution. There is stagnation/re-circular region on the wall opposite to the exhaust where the off-gas fraction is maximum.
Right: Temperature in fiber tow bands. Temperature is non-uniform due to different radiation heating in different furnace compartments and single exhaust location.

Conclusions

- We have developed a computational model for the CF LT furnace.
- Model can be used to analyze steady state and transient conditions, and can be extended to other furnace types and processing conditions.
- Model couples large scale effects (CFD) with fiber conversion process (thermochemistry)-Disparity in length and time scales requires HPC.
- The model is implemented in the open source software.