Develop a Simulation Framework for Understanding Physico-Chemical Processes and Optimization of CHZ' Plastic Thermolyze Technology

Cooperative Research and Development Final Report

CRADA Number: CRD-20-17273

NREL Technical Contact: Hariswaran Sitaraman

NREL is a national laboratory of the U.S. Department of Energy
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Cooperative Research and Development Final Report

Report Date: July 8, 2025

In accordance with requirements set forth in the terms of the CRADA agreement, this document is the CRADA final report, including a list of subject inventions, to be forwarded to the DOE Office of Scientific and Technical Information as part of the commitment to the public to demonstrate results of federally funded research.

Parties to the Agreement: CHZ Technologies LLC

CRADA Number: CRD-20-17273

CRADA Title: Develop a Simulation Framework for Understanding Physico-Chemical Processes and Optimization of CHZ' Plastic Thermolyze Technology

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Sponsoring DOE Program Office(s):

Office of Energy Efficiency and Renewable Energy (EERE), Advanced Manufacturing and Materials Technologies Office

JWS Funding Table showing DOE funding Commitment:

Estimated Costs	Contractor In-Kind	Participant In-Kind	Funds-In	Totals
Year 1	$300,000	$75,000	$0	$375,000
TOTALS	$300,000	$75,000	$0	$375,000

Executive Summary of CRADA Work:

Thermolyzer™ technology is a third-generation, multi-reactor, oxygen-free, low pressure, slow pyrolysis process. It has proven to be remarkably versatile in successfully processing all types of hydrocarbon waste. These include all seven types of plastics, tires, auto shredder residue, carpet, electronic waste, and composites. Working with the IACMI, Thermolyzer™ technology has recovered the glass and carbon fibers from wind turbine blades for reuse into new applications. Its primary output is a synthesis gas that is rich in H_2, CH_4, and small amounts of C_{2-4} aliphatic hydrocarbons. Other components are CO and CO_2. Three unique features set Thermolyzer™ apart from other pyrolysis systems: the syngas is clean enough to run in Siemens or Solar gas turbines or IC engines without fouling, clean, salable, byproducts are produced, and CO_2 emissions are lower than natural gas power plants. Research results have been obtained from an operating 7 ton/day facility. A 44 ton/day plant has successfully operated as noted above. The process works because it makes use of the recoverable embodied energy in the feedstock.

Surprisingly, a pound of some plastics has the same recoverable energy content as a pound of gasoline. Thus, it is imperative to develop a process that economically converts scrap plastics (including ocean plastics) into energy and thereby conserve the non-renewable fossil fuels for future generations. The Thermolyzer™ technology can also be used to create liquid fuels like gasoline and diesel from hydrocarbon wastes. Because of the high hydrogen content of the synthesis gas, hydrogen can be recovered more inexpensively than the current solar or wind energy being used to electrolyze water. That hydrogen can be used for fuel cell powered vehicles or converted into ammonia for agriculture or as a hydrogen storage medium. Extension of this technology to other wastes such as tires, auto shredder residue or wood wastes would expand the circular economy.

CRADA benefit to DOE, Participant, and US Taxpayer:

- Assists laboratory in achieving programmatic scope
- Enhances the laboratory's core competencies
- Enhances U.S. competitiveness by utilizing DOE developed intellectual property and/or capabilities.

Summary of Research Results:

Introduction

The primary issues that limit the size of the Thermolyzer™ technology are the complex material flow patterns due to the internal geometry of the reactor, temperature gradients, heat transfer to and from the reacting feedstock, ongoing chemical reactions, and the interactions with the emitted gases in the multiple reactors. Specifically, the input material is shredded to <5 cm size and goes into the top of the primary reactor operating at about 10 mbar pressure. There is a temperature gradient top to bottom of the reactor which has a complex shape. The material moves both radially and vertically in the reactor. Conventional CAD modeling programs are insufficient to handle the complex variables of heat transfer, chemical conversion of the feedstock, heat transport by the reacting materials and the transport of the feedstock intermediate product gas. In addition, the process creates pyrolysis oils and tars which are removed, separated from the syngas and returned to a secondary reactor to create more syngas. The problem varies with the input material, as tires are different from most plastics, etc.

Specifically, the discrete element method is typically used for modeling the impact of forces such as gravity on the transport process or modeling forces that can be derived from material data. This can be adopted for thermolysis, but the following points should be considered: the bulk material is subject to dynamic changes due to compression, chemical reaction and agglomeration. Particles down to the nano range are formed. (The particle sizes and composition have an impact on the reaction because they are not only reaction partners but also act as catalysts). Secondly, the flow behavior of the bulk material is also affected by forces resulting from the adhesion of the particles because they are melting. Additionally, in the boundary layer close to the wall (higher temperature), additional forces act, which result from the processes of material and heat transfer. The entire process of mass and heat transfer and the reaction processes are dynamic in space and time.

The reaction can basically be described mathematically, but there are many equilibrium reactions of various substances which take place competitively with unknown beginning and time course etc. The mass and heat transfer leads to a considerable dynamic of the entire process composed of several reactions. Furthermore, it is an open system in which components evaporate and gasify and participate in the reaction with their properties and also their functions (e.g., catalytic) or are gone and do not participate.

At present, we believe that only about 65% of the variables are being handled by the design programs. While this limitation is not too important for a small R&D facility, it becomes crucial in designing an 88 ton/day unit or a 176 ton/day unit. Commercial programs such as Solidworks or Ansys for design and Molecular Workbench or My Chemistry Laboratory for chemical reaction modeling are simply unable to handle all the required parameters, hence the need for high performance computing These are the commercial size units that can solve the plastic, tire and auto shredder wastes that are filling landfills. It is not possible to design such machines with the certainty they will work effectively from the start. That is why HPC is essential to the future success of this unique technology for helping solve the waste issues in the world and produce energy that conserves non-renewable natural resources economically and competitively. The key NREL capabilities that will be brought to bear to solve this problem are the high-performance computing technologies that can handle extremely large mesh sizes and can include conditions like those noted above. HPC is essential to solve this complex multi-phase dynamic process.

Approach

The approach is to use a multi-fluid model that resolves the gas, plastic feedstock particles and molten material as interpenetrating continuous phases. Previous capabilities developed at NREL on continuum-based modeling of biomass feedstock flows in hoppers and screw feeders was leveraged. The multi-fluid solver will be primarily developed on top of open-source Computational-Fluid- Dynamics (CFD) library, *OpenFOAM*, as has been previously done by the team at NREL in biomass feedstock flow (gas-solid) and gas-fermentation (gas-liquid) modeling. The *multiPhaseEulerFoam* solver that comes along with *OpenFOAM* library will be our starting point on which some of the custom models pertaining to solid-phase transport and chemistry will be implemented. We also used our in-house developed discrete-element-method solver that is amenable to large scale computing for solving few cases with high solids loading.

Results and discussion

TASK 1: IMPLEMENTATION OF ADDITIONAL PHYSICS INTO EXISTING SOFTWARE

Activities:

1. Implement polydispersity and specific drag/heat-transfer models for plastic particles.
2. Implement phase-change and melt rheology physics.
3. Implement conjugate heat-transfer through the screw.

Deliverables:

1. NREL will implement the above features into their software framework. It is noted that this deliverable is contingent on CHZ providing the required data and or material.
2. CHZ will provide measurements of physical parameters pertaining to liquid phase material.

Milestone 1:

1. A non-reacting flow simulation that provides a qualitative description of material flow and heat-transfer in the Thermolyze (NREL).
2. Viscosity and density measurements of tar and pyrolysis oils (CHZ)

Implementation of Additional physics into existing software

Although we lacked experimental data to allow for concrete comparisons of the rheology characteristics of the solids, we were able to estimate some of the important quantities affected by the rheology like the necessary torque required to mix the bed of solids. We also implemented a height-depending heat flux boundary condition to account for non-uniform heating from the burners outside of the reactor. We used open-source software, OpenFOAM, for this task. First, the OpenFOAM framework has a complete implementation of particle-particle interaction via the kinetic theory of granular flows. The equations of motion are described in a multiphase Eulerian framework for mass, momentum, and energy exchanges between phases.

Figure 1(a) shows the temperature distribution and granular flow streamlines towards the bottom of the reactor. The screw convey enables top-down mixing and mitigates temperature heterogeneities from non-uniform surface heating from the burners. A study of torque dependence on size of screw was studied using two different configurations of screws at the baseline diameter and a 50% larger diameter. Figure 1(b) shows the difference in torques, the steady state torque with the larger screw increases by 2.5 times with only 1.5X change in diameter. This can be attributed mainly to increase in surface area, although larger screw only marginal improvement in top-down mixing.

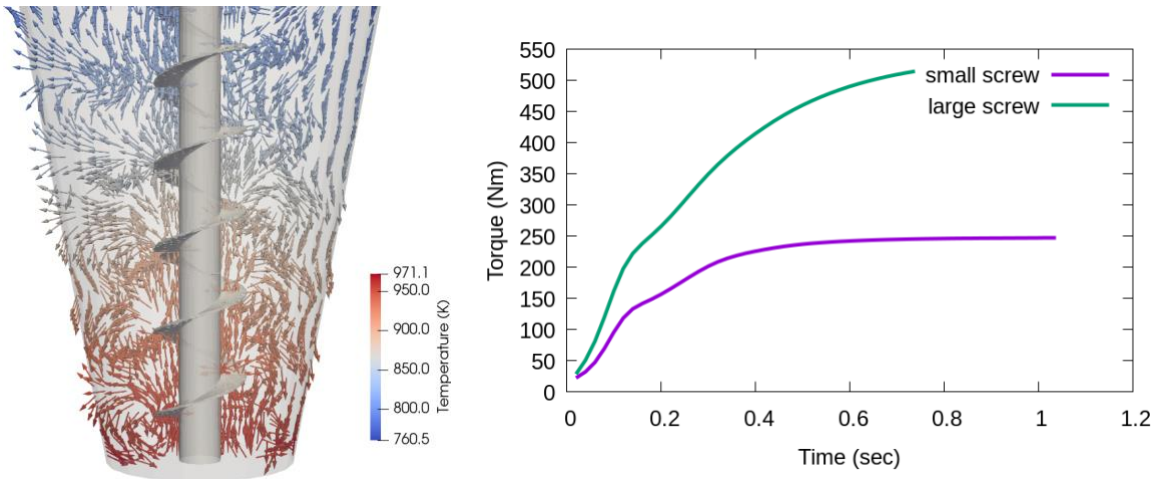


Figure 1. Estimation of torque based on shear stress from numerical simulations

Detailed and lumped mechanisms for the decomposition of biomass and plastic wastes have been described in the literature[1,2] Plastics feedstocks include Polyethylene (PE), Polyethylene terephthalate (PET) and Polystyrene (PS). An inherit advantage of the lumped mechanisms is their low computational cost considering that special methodologies are needed too couple kinetic and fluid-dynamic calculations. Figure 3 shows the main mechanisms for biomass and plastics thermal decomposition.

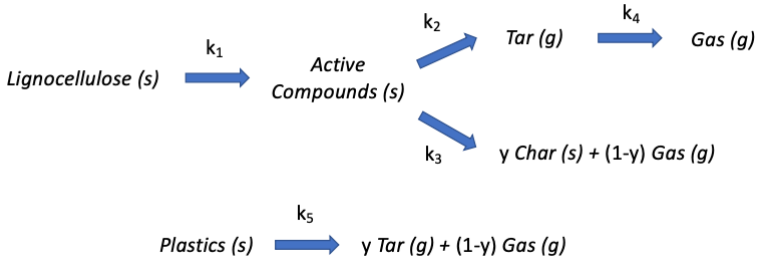


Figure 2. Lumped kinetic mechanisms for bio-waste decomposition.

In these mechanisms, each major component undergoes first order reactions that result in different compositions of bio-tar, non-condensable gases, and bio-char. Each component has its own temperature-dependent reaction rate represented by Arrhenius-like expressions for first order kinetics of the form:

$$k_i = A_i T_P^{\beta_i} \exp\left(\frac{-E_i}{RT_p}\right),$$

where A_i and E_i are the pre-exponential factor and activation energy for the reactions. Table 1 lists the reactions and reaction rates.

Table 1. reactions and reaction rates.

Type	Reaction	Pre-exponential factor A_i (s^{-1})	Activation Energy E_i $(MJkmol^{-1})$	Char formation ratio y_i
Cellulose	Cell $\xrightarrow{k_{c,1}}$ Acell	2.8e9	242.4	–
	Acell $\xrightarrow{k_{c,2}}$ Tar	3.28e14	196.5	–
	Acell $\xrightarrow{k_{c,3}}$ y Char $+ (1-y)$ Gas	1.3e10	150.5	0.35
Hemicellulose	Hemi $\xrightarrow{k_{h,1}}$ Ahemi	2.1e16	186.7	–
	Ahemi $\xrightarrow{k_{h,2}}$ Tar	8.75e15	202.4	–
	Acell $\xrightarrow{k_{h,3}}$ y Char $+ (1-y)$ Gas	2.6e11	145.7	0.60
Lignin	Lig $\xrightarrow{k_{l,1}}$ Alig	9.6e8	107.6	–
	Alig $\xrightarrow{k_{l,2}}$ Tar	1.5e9	143.8	–
	Alig $\xrightarrow{k_{l,3}}$ y Char $+ (1-y)$ Gas	7.7e6	111.4	0.75
Tar	Tar $\xrightarrow{k_{tar}}$ Gas(CO_2, CO, H_2, CH_4)	4.25e6	108	–
Heterogeneous reactions	$C + CO_2 \xrightarrow{kt_{CO_2}} 2\,CO$	2.68e4	589	–
	$C + H_2O \xrightarrow{kt_{H_2O}} CO + H_2$	2.68e4	589	–
	$C + 2\,H_2 \xrightarrow{kt_{H_2}} CH_4$	2.68e4	0.589	–
Homogeneous reactions	$CO + H_2O \xrightarrow{kh_{CO}} CO_2 + H_2$	1.51e3	2.780	–
	$CH_4 + H_2O \xrightarrow{kh_{CH_4}} CO + 3\,H_2$	3.0e8	–	–

[1] Ding, et. al., CFD simulation of combustible solid waste pyrolysis in a fluidized bed reactor. (2020). *Powder Technology*, 362, 177–187

[2] Ranzi, et. al., Chemical Kinetics of Biomass Pyrolysis. (2008). *Energy & Fuels*, 22, 4292–4300

In addition to the lumped mechanisms for biomass and plastic decomposition, we have also implemented additional kinetic steps, related to the cracking of tar into non-condensable gases (CO_2, CO, H_2, CH_4). The char species also undergo further gasification through reactions with CO_2, H_2O and H_2. Steam reforming of methane and water gas shift reactions are also added which are active at higher temperatures (~ 600 C).

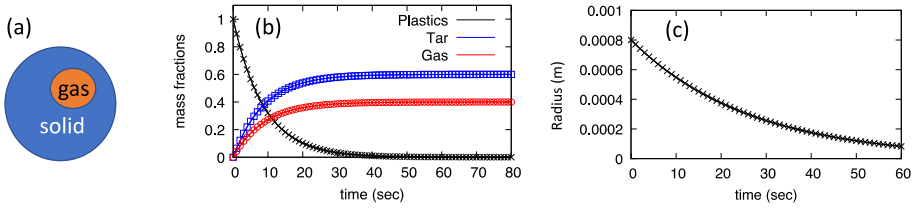


Figure 3: (a) schematic of solid plastic particle converting to gas, (b) and (c) species mass fractions and particle radius as a function of time from simulation (symbols) compared against analytic solution (solid line).

Furthermore, we developed a chemistry update feature within our in-house open-source discrete-element-method (DEM) code BDEM (https://github.com/NREL/BDEM), for high fidelity Lagrangian simulations of feedstock pyrolysis at high solids loading conditions. The chemistry solve at the particle scale assumes that each particle consists of a solid and a gas volume fraction as shown in Figure 3(a). The chemical species exists in both the solid and gaseous phase and are represented in the form of mass fractions. Solids to gas phase conversion is modeled as a rate of reduction in particle radius. The following ordinary differential equations for chemistry are solved alongside particle position and velocity update in our discrete-element-method:

$$\frac{d}{dt}(\bar{\rho} Y_{si} V) = -\dot{r}_i \tag{1}$$

$$\frac{d}{dt}\left(\bar{\rho} Y_{gi} V\right) = \dot{r}_i \tag{2}$$

$$\frac{d}{dt}(\epsilon_s \rho_s V) = \sum -\dot{r}_i \tag{3}$$

Where $\bar{\rho}$ is the average particle density, Y_{si} and Y_{gi} are the gas and solid species fraction for species i. V is the volume of the particle, ϵ_s is the solid volume fraction, ρ_s is the solids density and $\dot{r}_i$ is the production rate of species i obtained from a simplified chemical mechanism for plastics feedstocks that include solid species (e.g. PE, PET, PS) conversion to gas phase Tar (or oils) and gas.

Additionally, the average density is calculated using gas volume fraction (ϵ_g) and solids volume fraction using equations below:

$$\epsilon_g = 1 - \epsilon_s \quad (4)$$

$$\bar{\rho} = \epsilon_g \rho_g + \epsilon_s \rho_s \quad (5)$$

Equation 3 can be further simplified assuming the solid density remains constant, and $V = \frac{4}{3}\pi r_0^3$ corresponds to the total volume of the particle with its initial radius r_0 and $\epsilon_s = r^3/r_0^3$ where r is the particle radius at time t. The modified solids volume fraction equation becomes:

$$\frac{d\epsilon_s}{dt} = \frac{\sum -\dot{r}_i}{V} \quad (6)$$

Figure 3(b) and (c) show a comparison of computed solution for a single particle against the analytic solution for PE conversion to Tar and gas. This single particle simulation therefore verifies our chemistry solver implementation to be used in multiparticle simulations.

TASK 2: VALIDATION WITH EXPERIMENTS

Activities:

1. Development of simplified chemical mechanism from literature.
2. Coupling of chemistry with the non-reacting flow solver.
3. Iterative fitting with CHZ's product composition data
4. Finalize geometry of the research reactor based on CHZ's inputs.

Deliverables:

1. NREL will develop a simplified chemical mechanism for plastic pyrolysis and couple it with the multiphase solver from task 1. It is noted that this deliverable is contingent on CHZ providing the required data and or material.
2. CHZ will provide product composition data report for fitting purposes at a specific plastic mass input and steam setting. The computational model will then be used to predict the product composition at a different setting which will be validated against CHZ's experiment.

Milestone 2:

1. Documented validation study demonstrating agreement within 10% for syngas production for a given solids, temperature, pressure and steam setting (NREL).

As part of the validation task for the CFD models we have incorporated experimental results from the literature specifically, for one of the most common systems in the thermal decomposition of biomass: the fluidized bed. The work of Xiong et. al.[3] describe the operation of a fluidization system for the pyrolysis of biomass. The dimensions of the reactor are 0.34 m in height and 0.038 m in diameter. The density of the biomass is 400 kg/m^3 with diameters in the range 2.5x10^{-4} m – 4x10^{-4} m. The feedstock is fed at a rate of 0.1 kg/h while fluidization gas (N2) is added from the bottom at a speed of 0.36 m/s. The fraction of cellulose, hemicellulose and lignin is 0.41, 0.32, and 0.27 respectively. An additional solid phase (silica) acts as a fluidization agent with density 2649 kg/m3 with particle size 5.2x10^{-4} m. The reactor is preheated at 773 K to provide enough energy for the pyrolysis reactions. We constructed 2D simulations of this system using the kinetic description from Ding described in the previous section. Figure 4 shows the profiles of volume fraction and mass fraction of the different yields of syngas, tar, and biomass.

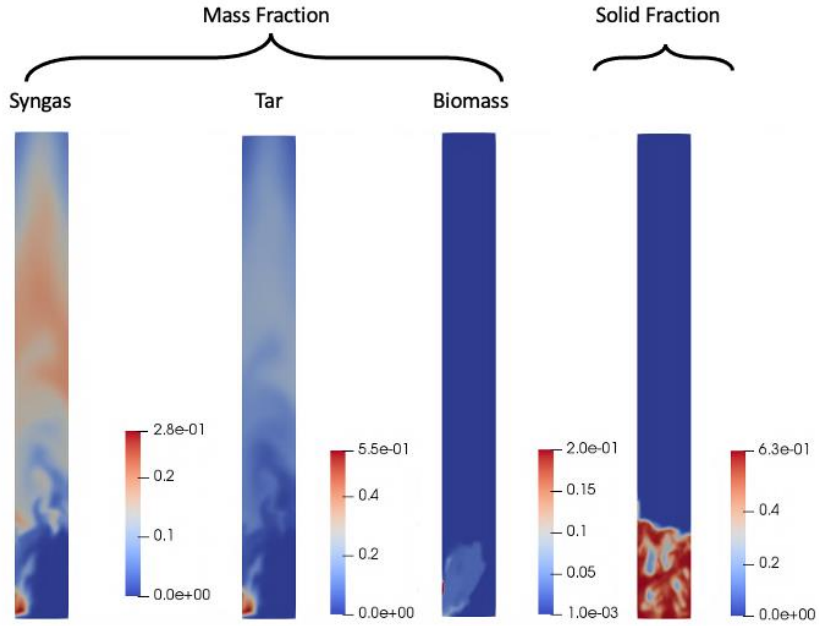


Figure 4. Mass and solid volume fraction profiles in fluidization system. As the pyrolysis progresses, tar and syngas are released into the gas phase.

The comparison against experimental data is summarized in table 2. Outlet averages of the last 30 seconds of simulation were taken for syngas, tar, and temperature, where the yields were renormalized by total mass of biomass. The results agree well with the experimental data, and the slight discrepancies are within the experimental uncertainty and the modeling approximations.

Table 2. Comparison of yields between experiments and simulations

	Syngas	**Tar**	**Temperature**
Experiment	20.5±1.3	71.7± 1.4	773
Simulation	22.7	68.9	780

[3] Xiong et. al., (2013). Development of a generalized numerical framework for simulating biomass fast pyrolysis in fluidized-bed reactors. Chem. Eng. Sci. 99, 305-313

TASK 3: PREDICTIONS FOR LARGE-SCALE REACTOR

Activities:

1. Finalize geometry and settings for large-scale reactor with information provided by CHZ.
2. Simulations of large-scale reactor at various settings providing sensitivities to input parameters.

Deliverables:

1. CHZ will provide reactor geometry and range of input settings for mass flow rate, temperature, pressure and steam concentration.
2. NREL will provide conversion sensitivities to these input settings. It is noted that this deliverable is contingent on CHZ providing the required data and or material.

Milestone 3:

1. Describes predictive simulations of large-scale pyrolysis reactors with sensitivity to input settings.

Optimization and scale-up studies

3.1 Optimization studies on small scale reactor

We used coupled transport and chemistry models in both Eulerian and Lagrangian frameworks to study CHZ's current reactor. Our aim was to obtain optimal temperatures and feedstock properties for maximizing value added products such as hydrogen and biochar while reducing CO2 production.

3.1.1 Discrete element method simulations

We performed DEM simulations using our in-house open-source software BDEM, which provides a Lagrangian description of solid flows. Lagrangian descriptions are useful because they represent particle-particle interaction and solid segregation with minimal modeling parameters. The main limitation is high computational costs associated with large number of particles present in current and scaled-up Thermolyzer™.

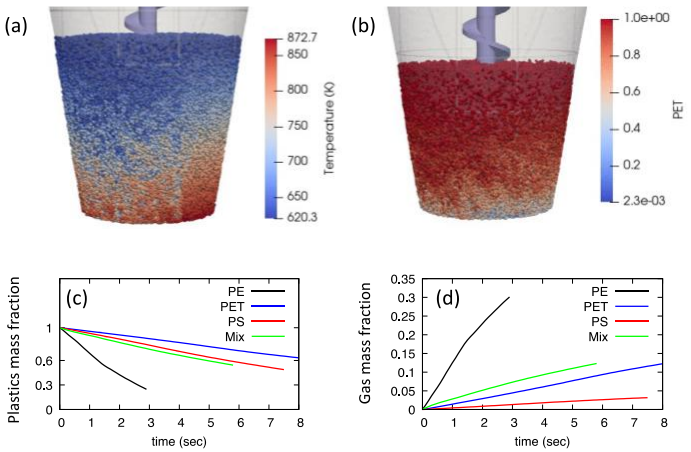


Figure 5: (a) shows temperature distribution in the reactor at early times t=0.05 sec, (b) shows PET mass fraction at time t=8 sec, (c) and (d) show reactor averaged plastics and gas mass fractions as a function of time.

Figure 5 shows simulation results from DEM simulations where we used 1 million 0.5 cm^3 particles. These simulations required 2 days of wall clock time on 200 processors on NREL's supercomputer, *Eagle*. Four cases were studied that include pure PE, PET, PS particles and a mixture case with each plastics feedstock at 33%. Figure 5 (a) shows the inhomogeneous temperature distribution in the particle phase due to non-uniform wall heating. Figure 5(b) shows a snapshot of the absolute PET mass fraction for a pure PET simulation at the end of 8 seconds of reaction time indicating higher conversion towards the bottom of the reactor where the temperatures are higher. The particle level is also lower compared to the initial distribution (Figure 5(a)) due to size reduction from conversion. Figures 5(c) and (d) show reactor averaged plastics and gas mass fractions which indicate that PE is easily pyrolyzed compared to PET and PS. PET is the slowest in terms of conversion. The mix feedstock case with equal distribution among PE, PET and PS (33% each) shows an intermediate conversion speed. This study indicates that conversion is feedstock dependent and tailoring the feedstock mixture can improve conversion speed. Figure 5 shows our further investigations on stratifying the feedstock with more reactive plastics towards the bottom of the reactor where the burner heating is dominant. The two cases studied in Figure 2 shows that having more reacting plastics in high temperature zones enables faster conversion. Higher rotational speeds enable greater top-down n mixing as illustrated in Figure 6 for the stratified case 1 from Figure 5. The PS conversion is higher with increased screw speed of 6 rad/s compared to 2 rad/s as shown in Figure 6(a) while PE conversion (Figure 6(b)) is reduced at higher rotational speed. Both these effects are due to increased mixing where more PS particles come down to higher temperature zones while PE particles start moving towards the top to lower temperature zones. There is no appreciable variation in overall gas conversion due to these competing effects from increased mixing, which makes the temperature distribution in the reactor the key towards improved conversion.

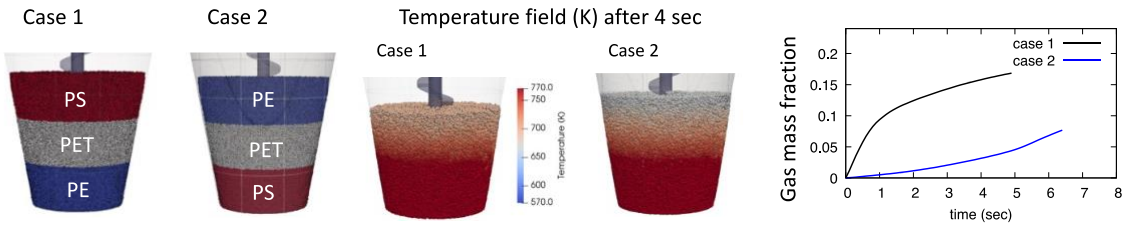


Figure 6: Study of stratifying feedstocks to achieve faster conversion. Case 1 has PE at the bottom while Case 2 has PE at the top. The temperature fields for case 1 and 2 indicate faster conversion for case 1 due to preferential heating of the reactor towards the bottom. The reactor averaged gas fraction production rate is higher for case 1.

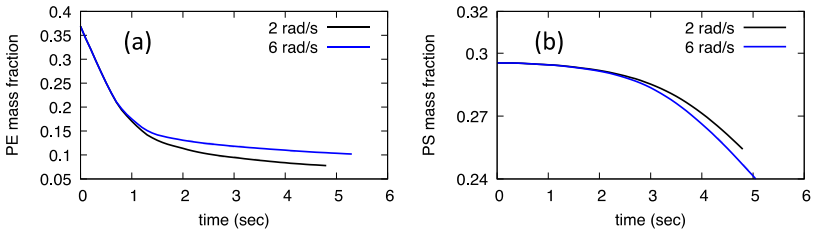


Figure 7: effect of screw rotational speed on (a) PE and (b) PS conversion for case 1 from figure 5.

3.1.2 Feedstock optimization for improved char production

CHZ was interested in variation of biochar production from various biomass feedstocks that contain varying cellulose, hemicellulose, and lignin content. We performed zero-dimensional chemistry simulations to probe feedstocks and optimize temperatures for higher char production. CHZ provides us with the cellulose, hemicellulose, and lignin fractions 8 feedstocks such as spruce, eucalyptus and walnut-shells. Our simulations predicted that walnut-shells with the highest lignin content provided the highest char yield as shown in Figure 8(a). Char yield also was found to exhibit a maximum at around 340 C that are similar to torrefaction temperatures as shown in Figure 8(b). Higher temperatures led to further gasification of char to light gas species such as CO and CO2.

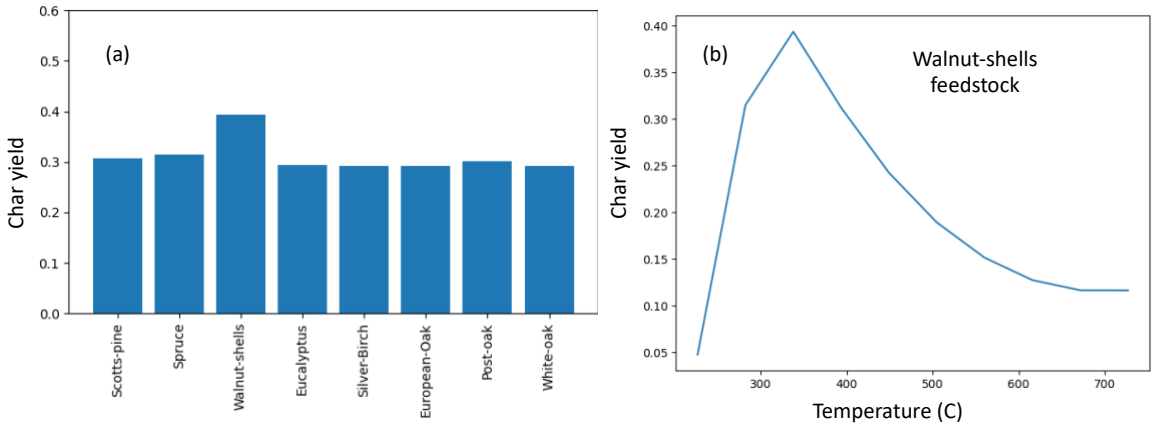


Figure 8: Char yield (mass of char over mass of biomass) for (a) varying feedstocks at 340 C and (b) for walnut-shells with varying temperature

3.2 Scaled up reactor simulations.

Complex interactions between the fluid-dynamics and the thermochemical decomposition govern the overall behavior of the thermal decomposition in the CHZ Thermolyzer™. A multiphase Euler-Euler model was used to study the effect of scaling up the reactor by 10 times. The effect of scaling the diameter of the reactor is shown in Figure 9 where the average solids temperature is shown as a function of time. It takes longer to heat the reactor from the heat flux from the burners on the reactor's lateral surface. The slower average temperature reduces the overall plastics conversion rate to syngas and oils.

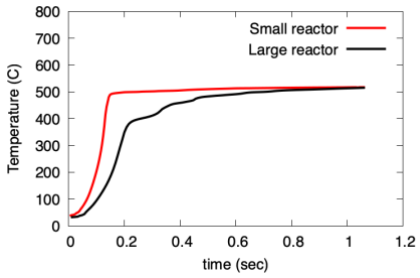


Figure 9: effect of reactor diameter on average solids temperature transients in the reactor. Temperature rise is slower with larger size.

Tasks	Milestones	Comments and variations	Timeline
1	A non-reacting flow simulation that provides a qualitative description of material flow and heat-transfer in the ThermolyzerTM.	We presented results from non-reacting flow simulation through presentations in internal biweekly meetings. Viscosity and density measurements of tar and pyrolysis oils was obtained from literature instead of CHZ experiments.	Scheduled time: month 4 Delivered time: month 4
2	Validation studies demonstrating agreement within 10% for syngas production for a given solids, temperature, pressure and steam setting.	NREL developed simplified chemical mechanism for plastic pyrolysis and coupled it with the multiphase solver from task 1 and an in-house open-source DEM solver. We validated our model against literature data on fluidized bed based pyrolysis and then performed validation study with CHZ's 7 ton/day reactor. Our results pertaining to CO2/CO/H2 yields matched well with CHZ's measurements. There was significant delay in delivering this milestone as NREL was short staffed and hiring was slow during COVID lockdown times.	Scheduled time: month 9 Delivered time: month 20
3	Predictive simulations of large-scale pyrolysis reactors with sensitivities to input settings.	Our simulations tested scaling up of thermolyzer to 10X capacity and showed increased diameter can affect heat transfer to feedstocks and in turn affect conversion.	Scheduled time: month 12 Delivered time: month 24

Issues or Challenges

The project was short staffed for a significant period with employee attrition at NREL and hiring delays during COVID lock down times. The milestone dates were extended along with the project period of 24 months.

Impact

The proposed work provided a framework to help CHZ Technologies advance its process in several ways that are in-line with the objectives of the HPC4EI/HPC4Mfg program, including accelerating design optimization, reducing experimental testing, and shortening time-to-adoption. The design and process improvements resulting from the CFD model demonstrated the possibilities of scale up studies and could greatly accelerate CHZ disruptive technology to commercial scale. This project supports the nations' goals on greenhouse gas emission reduction and supports a circular economy for waste plastics, biomass and municipal solid waste. Without this model, technology development will progress by time-consuming trial-and-error experiments, resulting in additional development cycles and less efficient, higher cost, sub-optimal designs.

Future Work

We hope to continue this work through HPC4EI phase 2 proposal or other opportunities through EERE BETO.

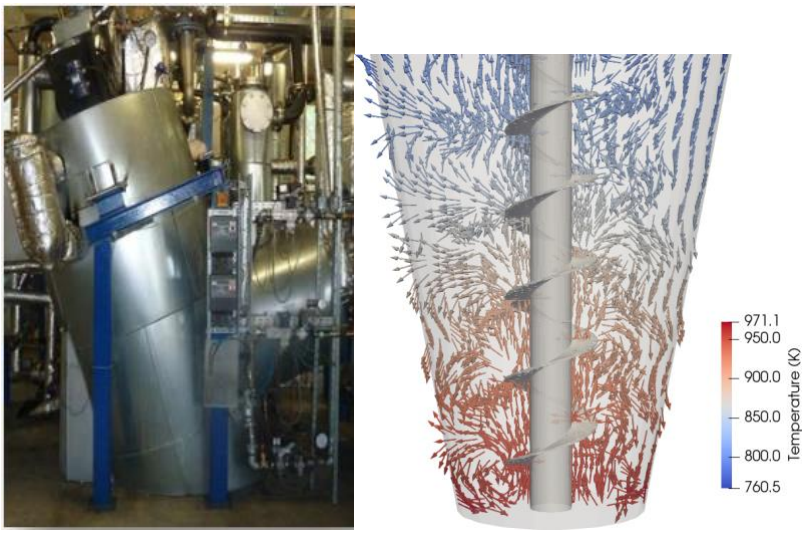
TASK 4: CRADA Report

Activities:

1. CHZ will assist NREL in the development of CRADA Report

This report serves to meet the requirements for the CRADA Final Report with preparation and submission in accordance with the agreement's Article X.

Pictures for Publication



(Left) shows CHZ's ThermolyzerTM and (right) shows a multiphase simulation of feedstock mixing and temperature distribution in the reactor.

Computational Resources used for Project:

System	Time (MCH)	Largest # of cores used	Commercial Software	Custom Software
Eagle	1.2 mill core hours	288		OpenFOAM

Briefly describe any algorithm development. How and to what extent will this development be disseminated internally and/or externally?

Some features were added to our open-source discrete-element-method solver which is now committed to the main branch of https://github.com/NREL/BDEM/. We presented our work at the international conference on Numerical Combustion:

Milo Parra-Alvarez, Hariswaran Sitaramana, Vivek Bharadwaj, Chuck T. Ludwig, Henry W. Brandhorst, Andreas Unger, Andreas Foerster, Development of an AI based tool for rapid assessment of pyrolysis yields from plastics and biomass mixtures, presented at 18th International Conference on Numerical Combustion, May 08, 2022 - May 11, 2022, San Diego, CA, USA

References:

None

Subject Inventions Listing:

None

ROI#:

None