CFD-Driven Optimization of a Bench-Scale Fluidized Bed Biomass Gasifier using MFiX-TFM and Nodeworks-OT

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Cover Illustration: Contours of the mass fraction of gaseous species generated in a biomass fluidized bed gasifier.


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<td>Computational fluid dynamics</td>
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<td>CI</td>
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<td>DOE</td>
<td>Design Of Experiments</td>
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<td>GP</td>
<td>Gaussian Process</td>
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<td>LH</td>
<td>Latin Hypercube</td>
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<td>MFiX</td>
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<td>RBF</td>
<td>Radial basis function</td>
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<td>RSM</td>
<td>Response Surface Model</td>
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ABSTRACT

Biomass is a widely available renewable energy source, which could be an alternative fuel source to fossil fuels to mitigate serious environmental problems. Gas-solid fluidized bed reactors offer excellent mixing, and heat and mass transfer between solid particles and a fluidizing gas. As such, a fluidized bed reactor is ideal for thermal/thermochemical conversion of biomass to valuable gas products. Despite many decades of research into improving the operation of biomass gasifiers, the process of biomass gasification is not yet well understood. Biomass gasification performance is strongly affected by operation conditions of the gasifier. Optimizing a reactor, such as a fluidized bed, experimentally is time consuming and expensive. Advancements in high performance computing, has made computer simulation a powerful tool for design engineers and decision makers. In this report, a bench-scale fluidized bed biomass gasifier is simulated using Multiphase Flow with Interphase eXchanges (MFiX) - two-fluid model (TFM). The Optimization Toolset (OT) in the National Energy Technology Laboratory’s (NETL) Nodeworks software is used to optimize the operation of the fluidized bed, such that the H₂ to CO ratio in the syngas is 2.0. This optimization is achieved by optimizing the biomass feedstock flow rate, mass flow rate of fluidizing gas, and the amount of steam in the fluidizing gas. The performance of the optimal operating condition—evaluated via a surrogate model—is tested through a final computational fluid dynamics (CFD) simulation, resulting in a syngas composition within the expected accuracy of the model.
1. **INTRODUCTION**

Global climate change and greenhouse gas emissions have been an increasing concern in the past few decades. Currently, global economic growth relies heavily on energy produced from fossil energy, e.g., coal, petroleum, and natural gas, and it is expected that the global energy consumption will continue to grow in the coming decades. Gasification technology is an efficient way to produce high quality syngas products that can be used directly in power generation or chemical production industries. Gasification of renewables, such as biomass, is an attractive alternative to coal gasification. Biomass is an important renewable source of energy, available in abundance worldwide, with the potential to mitigate our reliance on fossil fuels for energy production. Although a byproduct of biomass gasification is CO$_2$, since biomass is a renewable source of energy, future growth of biomass material will offset the production of CO$_2$ as the result of gasification (www.netl.doe.gov/research/coal/energy-systems/gasification/gasifipedia/biomass).

Fluidized bed gasifiers have many desirable features, including: producing low tar syngas, maintaining uniform radial temperature distribution, preventing the formation of slag and the operational flexibility (Karimipour et al., 2013). Biomass gasification inside a fluidized reactor is extremely complicated, coupling mass, momentum, heat and mass transfer with chemical reactions. Hence, the gasification performance is strongly affected by operating conditions.

Optimization of the fluidized bed reactor is a time consuming and expensive process experimentally. Computational fluid dynamics (CFD) is a powerful simulation tool in modeling the performance behavior of a gasifier. Higher-fidelity multiphase CFD methods such as direct numerical simulation and CFD-discrete element method are computationally intensive and thus impractical for modeling of large-scale reactors. The two-fluid model (TFM) remains the practical simulation method for simulating large-scale gasifiers (Xue and Fox, 2014). In the TFM, a continuum description is employed for both the solid and gas phases. While the TFM is capable of predicting flow behavior of gas-solid systems at large scale, it relies on many closure relations, namely effective solids pressure and viscosity (Lun et al., 1984), affecting the accuracy of the results.

In this work, a numerical experiment is carried out to demonstrate the capabilities of the Optimization Toolset (OT) recently developed in the Nodeworks graphical programming library. A bench-scale fluidized bed gasifier is simulated using Multiphase Flow with Interphase eXchanges (MFiX)-TFM. A design of experiments is constructed in Nodeworks for a parametric space, where biomass flow rate, fluidizing gas flow rate, and steam content of the fluidizing gas vary. Simulation results are used to construct a spatially continuous response surface, i.e., a CFD data fitted surrogate model. The surrogate model is then used to determine the optimum operating condition that produces H$_2$ to CO ratio of two in the product syngas. Lastly, a single simulation at the optimal operating condition is performed as a check of the optimization process.
2. METHODS

2.1 SIMULATION METHODS

This study used TFM simulations of the open-source Multiphase Flow with Interphase eXchanges (MFiX) code available from the U.S. Department of Energy (DOE), National Energy Technology Laboratory (NETL) (https://mfix.netl.doe.gov). MFiX is a general-purpose computer code for modeling the hydrodynamics, heat transfer, and chemical reactions in fluid-solids systems (Xu et al., 2017a, 2017b, 2017c, 2019; Lu et al., 2018).

The TFM, or, more generally, the multi-fluid continuum model, treats both gas and solid phases in an Eulerian frame of reference as continuous and fully interpenetrating. The equations employed are a generalization of the averaged Navier-Stokes equations for interpenetrating continua which describe the conservation of mass, momentum, and energy. The governing equations can be derived from different averaging approaches such as volume averaging, time averaging, and ensemble averaging. In principle, the two-fluid model can be derived for different multiphase flow systems such as gas-liquid, gas-solid, etc., provided that proper closures are used to describe the rheology for each phase as well as the interfacial interactions.

The governing equations are summarized in this section for gas-solid flows in typical fluidized bed applications. In the two-fluid model, the phasic volume fractions, which are continuous functions of space and time, are introduced to track the volume fraction occupied by gas and solids. The volume fractions must sum to one, i.e.,

\[
\varepsilon_g + \varepsilon_s = 1 ,
\]

where \(\varepsilon_g\) and \(\varepsilon_s\) are the volume fractions of gas and solid phases, respectively. The gas phasic volume fraction is also known as the void fraction or voidage.

The continuity equations for gas and solid phases are

\[
\frac{\partial \varepsilon_g \rho_g}{\partial t} + \nabla (\varepsilon_g \rho_g \mathbf{u}_g) = -r_{gs} , \tag{2}
\]

and

\[
\frac{\partial \varepsilon_s \rho_s}{\partial t} + \nabla (\varepsilon_s \rho_s \mathbf{u}_s) = r_{gs} , \tag{3}
\]

where \(\rho_g\) and \(\rho_s\) are the gas- and solid-phase densities, \(\mathbf{u}_g\) and \(\mathbf{u}_s\) are the gas- and solid-phase velocities, and \(r_{gs}\) is the mass-transfer rate from gas phase to solid phase due to chemical reactions or physical processes such as evaporation. All flow field variables here are averaged quantities according to the averaging approach, i.e. time average, space average, or ensemble average.

The momentum equations for gas and solid phases are

\[
\frac{\partial}{\partial t} \varepsilon_g \rho_g \mathbf{u}_g + \nabla (\varepsilon_g \rho_g \mathbf{u}_g \mathbf{u}_g) = \nabla \sigma_g - \mathbf{f}_{gs} + \varepsilon_g \rho_g \mathbf{g} - \mathbf{m}_{gs} , \tag{4}
\]

and
\[
\frac{\partial}{\partial t} \varepsilon_s \rho_s u_s + \nabla (\varepsilon_s \rho_s u_s u_s) = \nabla \sigma_s + f_{gs} + \varepsilon_s \rho_s g + m_{gs}, \quad (5)
\]

where \(\sigma_g\) and \(\sigma_s\) are gas- and solid-phase stress tensors, \(f_{gs}\) is the interfacial interaction force between gas and solid phases, \(g\) is the gravity vector, and \(m_{gs}\) is the momentum transfer due to the mass transfer between phases.

The interaction force between two phases can be further divided into pressure gradient force and drag force in the following equation:

\[
f_{gs} = \varepsilon_s \nabla P_g + \beta_{gs} (u_g - u_s). \quad (6)
\]

The first term in the right side of Equation (6) for pressure gradient force is explicitly resolved by the model whereas the second term, the generalized steady drag force, is closed with the drag correlation. Here, the Gidaspow drag model (Ding and Gidaspow, 1990) is used, which is a combination of the Wen and Yu model in dilute \((\varepsilon_s < 0.2)\) regions and the Ergun equation in dense regions.

The energy balance for the gas phase, written in terms of the gas-phase temperature, \(T_g\), is:

\[
\varepsilon_g \rho_g C_{pg} \left( \frac{\partial T_g}{\partial t} + u_g \nabla T_g \right) = -\nabla q_g - Q_{gs} - \Delta Q_{rg} + Q_r, \quad (7)
\]

where \(C_{pg}\) is the gas-phase heat capacity, \(q_g\) is the gas-phase conductive heat flux, \(Q_{gs}\) describes the interphase heat transfer between gas and solid phases, and \(\Delta Q_{rg}\) is the heat of reaction partitioned to the gas-phase. The last term, \(Q_r\), accounts for heat transfer due to radiation. In Equation (7), the energy source terms due to viscous dissipation and interphase momentum transfer have been neglected as they are typically insignificant in most practical reacting fluidized bed applications.

Similarly, the energy balance equation for the solid-phase is:

\[
\varepsilon_s \rho_s C_{ps} \left( \frac{\partial T_s}{\partial t} + u_s \nabla T_s \right) = -\nabla q_s + Q_{gs} - \Delta Q_{rs} - Q_r, \quad (8)
\]

where \(T_s\) is the solid-phase (molecular) temperature, \(C_{ps}\) is solid heat capacity, \(q_s\) is the solid-phase conductive heat flux, \(\Delta Q_{rs}\) is the heat of reaction partitioned to the solid-phase, and \(Q_r\) is the radiation heat transfer from the solid phase to the gas flow. For heterogeneous chemical reactions taking place at the surface of the catalyst or fuel particles in fluidized bed reactors, it is important to distribute the heat of reaction properly. In MFiX, the user can either assign the heat of reaction to the specific phases or MFiX will assign the heat of reaction to the appropriate phases (mfix.netl.doe.gov/doc/mfix/latest).

The gas and solids phases may contain an arbitrary number of chemical species. The transport equation for each \(i^{th}\)-species is:
\[ \frac{\partial \varepsilon_g \rho_g X_{gl}}{\partial t} + \nabla (\varepsilon_g \rho_g X_{gl} u_g) = \nabla (D_{gl} \nabla X_{gl}) + R_{gl} \]  \hspace{1cm} (9)

or

\[ \frac{\partial \varepsilon_s \rho_s X_{sl}}{\partial t} + \nabla (\varepsilon_s \rho_s X_{sl} u_s) = \nabla (D_{sl} \nabla X_{sl}) + R_{sl} \]  \hspace{1cm} (10)

depending on whether the \(i\)-th species belongs to the gas- or solid-phase. In Equations (9) and (10), \(X_{gl}\) and \(X_{sl}\) are species mass fractions, \(D_{gl}\) and \(D_{sl}\) are diffusivities, and \(R_{gl}\) and \(R_{sl}\) are the rates of formation of gas and solid species.

2.2 REACTION KINETICS

The primary chemical processes that take place during biomass gasification are: drying, pyrolysis, gasification, and combustion. Wet biomass particles are initially heated by the surrounding gas and inert sand particles which leads to evaporation of moisture inside biomass particles.

\textbf{Drying: Moisture} \rightarrow \textbf{H}_2 \textbf{O} \hspace{1cm} (11)

The drying rate of moisture (kmole/m\(^3\)-s) is given as:

\[ r_1 = 5.13 \times 10^6 \times \exp\left( -\frac{10585}{T_p} \right) \times C_{\text{Moisture}} \]  \hspace{1cm} (12)

After drying is completed, the volatile matter inside the biomass is decomposed into char and volatile gases. In this work, the one-step global-reaction scheme of Liu et al. (2016) is used,

\textbf{Devolatilization: Volatiles} \rightarrow 5.96 \times \text{CO} + 2.95 \times \text{CO}_2 + 8.26 \times \text{H}_2 + 1.5 \times \text{CH}_4 + 0.5 \times \text{C}_2\text{H}_4 + 8.41 \times \text{Char} \hspace{1cm} (13)

The devolatilization rate of the volatile matter (kmole/m\(^3\)-s) is

\[ r_2 = 1.49 \times 10^4 \times \exp\left( -\frac{1340}{T_p} \right) \times C_{\text{Volatiles}} \]  \hspace{1cm} (14)

Once the volatile matter in the biomass is released into the gas stream, the remaining char in the biomass undergoes the heterogenous oxidation process. In this case, the oxidation agents are oxygen, steam, carbon dioxide, and hydrogen in the gas stream. Carbon oxidation with oxygen is modeled using the shrinking core model proposed by Syamlal and Bissett (1922),

\textbf{Char combustion: Char+O}_2 \rightarrow \textbf{CO}_2 \hspace{1cm} (15)

The rate of char oxidation (kmole/m\(^3\)-s) is given by

\[ r_{\text{char}} = \frac{-3 \varepsilon_s \rho_{O_2}}{d_p (k_{\text{film}}^{-1} + k_{\text{ash}}^{-1} + k_{\text{reaction}}^{-1})MW_{O_2}} \]  \hspace{1cm} (16)

where
\[ k_{film} = \frac{D_{O_2} \, Sh}{d_p \, T_R / MW_{O_2}}, \quad (17) \]

is the resistance due to film diffusion,

\[ k_{ash} = \frac{2r_d D_{eff, ash}}{d_p \, (1 - r_d) \, T_R / (MW_{O_2})}, \quad (18) \]

is the resistance due to ash diffusion, and

\[ k_{reaction} = A_{\text{char oxidation}} \, r_d^2 \, e^{-E_{\text{char oxidation}}/RT_s} \quad (19) \]

is the surface reaction resistance.

In Equation (19), \( A_{\text{char oxidation}} \) and \( E_{\text{char oxidation}} \) are given by Field et al. (1967) as 8,710 (gm/atm-cm\(^2\)-s) and 35,700 (cal/g-mole) respectively. Char oxidation with steam, carbon dioxide and hydrogen, which are also referred to as steam gasification, CO\(_2\) gasification and hydrogen gasification, take place according to the model of Syamlal and Bissett (1992). The steam gasification reaction is given by

\[
\text{Steam gasification: } \text{Char} + H_2O \rightleftharpoons CO + H_2, \quad (20)
\]

where the forward and backward gasification rates are

\[ r_{H2O_F} = 465000 \times \exp\left(-\frac{188280}{RT_{film}}\right) \times C_{\text{char}} \times P_{H_2O}, \quad \text{and} \]

\[ r_{H2O_R} = 465000 \times \exp\left(-\frac{188280+324}{RT_{film}} \times 17.29\right) \times C_{\text{char}} \times P_{H_2} \times P_{CO}, \quad (21) \]

respectively. The CO\(_2\) gasification reaction is

\[
\text{CO2 Gasification: } \text{Char} + CO_2 \rightleftharpoons 2CO, \quad (22)
\]

where the forward and backward gasification rates are

\[ r_{CO2_F} = 372000 \times \exp\left(-\frac{188280}{RT_{film}}\right) \times C_{\text{char}} \times P_{CO_2}, \quad (23) \]

and

\[ r_{CO2_R} = 372000 \times \exp\left(-\frac{188280+4030}{RT_{film}} \times 20.92\right) \times C_{\text{char}} \times P_{CO_2}^2, \quad (24) \]

respectively. The H\(_2\) gasification reaction is

\[
\text{H2 Gasification: } \text{Char} + 2H_2 \rightleftharpoons CH_4, \quad (25)
\]

where the forward and backward gasification rates are
\[ r_{\text{H}_2\text{F}} = \exp\left(\frac{-80.7}{T_{\text{film}}} - 7.087\right) \times C_{\text{char}} \times P_{\text{H}_2}, \]  

(26)

and

\[ r_{\text{H}_2\text{R}} = \exp\left(\frac{-135.5}{T_{\text{film}}} - 0.372\right) \times C_{\text{char}} \times P_{\text{CH}_4}^{0.5}, \]  

(27)

respectively. The homogenous oxidation of carbon dioxide with oxygen is

**CO combustion:** \( \text{CO} + \frac{1}{2} \text{O}_2 \rightarrow \text{CO}_2, \)

(28)

with a reaction rate of

\[ r_7 = 3.98 \times 10^{14} \times \exp\left(\frac{-201}{T_g}\right) \times \varepsilon_g \times C_{\text{O}_2}^{0.25} \times C_{\text{CO}} \times C_{H_2O}^{0.5}. \]  

(29)

The homogenous oxidation of methane with oxygen is

**CH4 combustion:** \( \text{CH}_4 + 2\text{O}_2 \rightarrow \text{CO}_2 + 2\text{H}_2\text{O}, \)

(30)

with a reaction rate of

\[ r_8 = 6.7 \times 10^{12} \times \exp\left(\frac{-24}{T_g}\right) \times \varepsilon_g \times C_{\text{CH}_4}^{1.3} \times C_{\text{O}_2}^{0.2}. \]  

(31)

The homogenous oxidation of hydrogen with oxygen is

**H2 combustion:** \( \text{H}_2 + \frac{1}{2} \text{O}_2 \rightarrow \text{H}_2\text{O} \)

(32)

\[ r_9 = 1.08 \times 10^{16} \times \exp\left(\frac{-151}{T_g}\right) \times \varepsilon_g \times C_{\text{O}_2} \times C_{\text{H}_2}. \]  

(33)

Finally, the water gas shift reaction is modeled as

**Water gas shift:** \( \text{CO} + \text{H}_2\text{O} \rightleftharpoons \text{CO}_2 + \text{H}_2 \)

(34)

where the forward and backward gasification rates are

\[ r_{10\text{F}} = 2.78 \times 10^{6} \times \exp\left(\frac{-1515}{T_g}\right) \times C_{\text{CO}} \times C_{H_2O}, \]  

(35)

and

\[ r_{10\text{R}} = 2.78 \times 10^{6} \times \exp\left(\frac{-1515}{T_g}\right) \times C_{\text{CO}_2} \times C_{\text{H}_2}/(2.9 \times 10^{-2} \times \exp(\frac{4094}{T_g})) , \]  

(36)

respectively.

### 2.3 SIMULATION SET-UPS

As stated earlier, the goal of this study has been to demonstrate the capabilities of the Optimization Toolset (OT) of the Nodeworks library to optimize the flow conditions for a biomass fluidized bed, such that \( \text{H}_2 \) to \( \text{CO} \) ratio in the syngas will be two. To this end, a bench-scale fluidized bed, shown in Figure 1, was used to carry out the numerical experiment. The
fluidized bed and the operating conditions are obtained from Sotacarbo Sustainable Energy Research Center, in Carbonia, Italy, through an ongoing collaboration. The fluidized bed consists of the lower mixing section, with a diameter of 26.65 mm and a freeboard region with a diameter of 53 mm. Biomass feedstock is injected at 90 g/h through a hopper via a screw feeder located at the lower side of the reactor. A small amount of N\textsubscript{2} at room temperature is injected to aid the feeding process at the rate of 1.943e-6 kg/s. The fluidizing gas is pre-heated up to 350 °C and injected through the bottom of the gasifier at the rate of 32.33e-6 kg/s. The bed material consists of 58 g of Olivine sand particles, to help with the fluidization of biomass particles and heat distribution in the bed.

![Figure 1: Schematic representation of experimental setup.](image)

The biomass used for the preliminary gasification tests is cypress from Sardinian woods. The proximate, ultimate and calorimetric analyses of this particular biomass is shown in Table 1. The analyses were carried out in the Sotacarbo laboratories according to international standards. More details on the calorimetric studies can be found in Porcu et al. (2019).
Table 1: Proximate and Ultimate Analysis of the Cypress Biomass Particles

<table>
<thead>
<tr>
<th>Proximate Analysis</th>
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<th>Ultimate Analysis</th>
<th>%</th>
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<tbody>
<tr>
<td>Fixed carbon</td>
<td>19.67</td>
<td>Carbon</td>
<td>51.97</td>
</tr>
<tr>
<td>Volatiles</td>
<td>67.14</td>
<td>Hydrogen</td>
<td>5.81</td>
</tr>
<tr>
<td>Moisture</td>
<td>10.78</td>
<td>Nitrogen</td>
<td>1.00</td>
</tr>
<tr>
<td>Ash</td>
<td>2.41</td>
<td>Sulfur</td>
<td>n.d.</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Oxygen</td>
<td>41.22</td>
</tr>
</tbody>
</table>

Figure 2: Properties of the Cypress biomass and Olivine sand particles.

A SympaTEC QICPIC particle analyzer was used to characterize the Cypress biomass and Olivine sand particles at NETL. Figure 2 shows the size distribution of the biomass and sand particles. In this study, the diameter of biomass and Olivine sand particles are assumed to be 1.06 mm and 202.2 µm respectively. The Cartesian grid cut-cell technique in MFiX is used to mesh the fluidized bed, with grid resolution of $11 \times 100 \times 9$ cells in $x$, $y$, and $z$-directions, respectively. The inlet is defined as a uniform mass flow inlet, with wall boundaries assumed to be no-slip, adiabatic walls.
3. **OPTIMIZATION**

3.1 **PROBLEM STATEMENT**

The goal of optimization is to achieve an optimal condition for the various input parameters to the process, such that a desired target in Quantities of Interest (QoIs) is reached. For the problem under consideration, this study assumes that:

- The gasifier is fluidized by a mixture of steam and air
- The syngas product is to be used by a downstream process which requires an ideal H₂ to CO ratio of two
- The optimal condition minimizes steam to biomass feedstock ratio

Stated mathematically, this study seeks to solve

\[
\min f = \frac{x_3 x_2}{x_1}, \quad y_1 = 2
\]

where \(x_i\) is the model input for each parameter, \(i\), and \(y_j\) is the system response quantity of interest (SRQoI). In this case, there is only one SRQoI, \(y_1 = H_2/CO\) (mole fraction), i.e., the molar fraction of hydrogen to carbon monoxide in the raw syngas. Three input variables are considered in this study: \(x_1 = \dot{m}_{\text{biomass}}\), the mass flowrate of the biomass feedstock, \(x_2 = \dot{m}_{\text{gas}}\), the mass flowrate of the inlet gas, a mixture of air and steam, where \(x_3 = X_{H_2O}\), the mass fraction of steam in the inlet gas.

3.2 **PRELIMINARY DOE SAMPLING**

Very little is known about the hypothetical reactor setup used in this study. Therefore, a rather coarse and broad sweep of the three-dimensional (3-D) input parameter phase space is considered in order to get a general feel for how the SRQoI is affected by the inputs. The biomass mass flowrate is \(2.5 \times 10^{-5}\) kg/s for the baseline simulation. Here, an interval of \(x_1\) from \(\frac{1}{4}\) to 4 times the base flowrate is considered. The fluidizing gas mass flowrate is \(3.2325 \times 10^{-5}\) kg/s. The \(x_2\) interval is taken to be \(2-10 \times 10^{-5}\) kg/s. The lower limit on \(x_2\) is kept rather tight to the baseline value to avoid accidentally de-fluidizing the system. The third and final input parameter essentially has no baseline value. The initial simulations were performed without steam being injected with the fluidizing gas. Therefore, a wide range of steam mass fraction in the fluidizing gas was taken as \(0 < x_3 < 0.5\).

The 3-D input parameter phase-space is sampled with 32 points. The sample points are generated with Nodeworks’ Design of Experiments (DOE) node. Due to the coarseness of the sampling, a space filling design is selected, specifically Latin Hypercube with optimization using the genetic algorithm. The variation of the sample points with respect to the three input parameters is visualized in Figure 3.
NETL’s Joule2 supercomputer was used to launch 32 MFiX simulations, based on the DOE generated by Nodeworks. Each simulation was launched on a single node, with 40 cores. With 4 to 5 days wall clock, 30 seconds of simulation time is achieved for each case. The species concentrations (molar fractions) are monitored at the system outlet. Figure 4 shows the time trace of the species mole fraction at the outlet, for the entire test matrix. Most cases reached the pseudo-steady state condition within the 30 seconds of simulation time. Although few simulations required more time to reach the pseudo-steady state condition, due to the computationally intensive nature of these simulations, it was determined that time-averaged quantities from 25 to 30 s would be sufficient for the present study.

The 5 s time average of the mole fraction ratio of H$_2$ to CO at the outlet is taken as the SRQoI $y_1$. The dependence in the SRQoI on the three input parameters can be discerned from the scatter plots of Figure 5. At this scale, it is difficult to observe much dependence in $y_1$ on $x_1$ and $x_2$ (mass flow rates of biomass and fluidizing gas, respectively). However, a strong dependence of $y_1$ on $x_3$ is clearly observable. The strong dependence of produced syngas composition on the steam content of the fluidizing gas was also observed in a previous experimental sensitivity analysis of coal gasification (Karimipour et al., 2013). Unfortunately, the range of H$_2$/CO ratio goes well beyond the target value of $y_2 = 2$. It should be noted that the observed ratios are potentially unrealistically high for biomass gasification, e.g., see Table 1 of Göransson et al. (2011); however, without data to validate and/or calibrate the model, it is difficult to make an accurate assessment. For the time being, the results are considered “as is” for this optimization study.
Figure 4: Transient plots of species’ molar concentration at the outlet for all 32 simulations of the initial DOE.
Figure 5: Scatter plots displaying the influence of the input parameters on the SRQoI.

Figure 6: Scatter plots displaying the influence of the input parameters on the SRQoI, highlighting region of interest $0 < y_1 < 5$.

Figure 6 shows the same scatter plots as shown previously in Figure 5, excluding all cases with a SRQoI above five. The reduced set still spans the full interval of $x_1$ and $x_2$; however, $x_3$ now only ranges up to approximately 20% (mass fraction). At this scale, some variation in $y_1$ on $x_1$ and $x_2$ appears. Although resampling beyond this preliminary phase-space sweep was anticipated, there is a noticeable gap in the data near the target design value $y_1 = 2$. Creating a surrogate with the available data would likely lead to significant error in approximating $y_1 = 2$ as a surface. In order to close this gap, additional samples are considered in the following section.

3.3 SECONDARY DOE SAMPLING

In this section, a second DOE is constructed in order to improve the ability of a surrogate model to capture the CFD-predicted behavior near $y_2 = 2$. Based on the preliminary study of the previous section, the ranges of $x_1$ and $x_2$ are increased slightly to $4-120 \times 10^{-6}$ kg/s and $1-12 \times 10^{-5}$ kg/s, respectively. The range of $x_3$, however, is significantly reduced, now restricted to 15% (mass fraction). The new phase-space is sampled with 51 points, again using Nodeworks’ DOE node with Latin Hypercube (LH) sampling optimized by the genetic algorithm.
The 51 new sample points are shown in orange in Figure 7. The new samples are simply added to the 13 points retained from the preliminary DOE with \( y_1 < 5 \) (in black in Figure 7). It should be noted that because each sample was generated individually, the corresponding 64 sample superposition is neither optimal (by any measure) nor even guaranteed to be a LH sample. This concession was made in order to reuse the results of the 13 previously completed simulations.

As before, 51 additional simulations are launched on 51 nodes of Joule 2. The new (orange) and previous (black) results are combined in the scatter plots of Figure 8. With the secondary DOE, there is now good coverage in the SRQoI around the design point, i.e., \( y_1 = 2 \).

**3.4 SURROGATE MODELING**

With samples in the input parameter phase-space with response values near the design condition, i.e., \( y_1 = 2 \), the process of optimizing the reactor, i.e., can begin by solving Equation (36). The most straightforward and, perhaps, the most obvious method is to directly iterate with the model: e.g., take the best condition of the 64 samples and resample locally, re-evaluate and re-sample until the change in the best condition reaches a defined tolerance and it is taken as the optimal
condition. However, since each (discrete) \( i \) model evaluation, \((x_1, x_2, x_3)_i \rightarrow (y_1)_i\), takes several days of simulation time, using the CFD model directly would be very computationally expensive and time consuming. To reduce computational costs of expensive CFD model evaluation, this study constructed a surrogate model to replace the full (CFD) model which is computationally inexpensive. Optimization will then take place on the surrogate which represents an approximate, continuous mapping of the input parameter phase-space to the output SRQoI.

A surrogate model is constructed using Nodeworks’ Response Surface Model (RSM) node. After initially testing several models two options, both leveraging radial basis functions (RBF), emerged as the best candidates: the RBF model with multi-quadratic functions (SciPy, 2019) and the Gaussian Process (GP) model with the \( 1^\text{st} \text{RBF} \) kernel using the \texttt{fmin_l_bfgs_b} optimizer with 10 restarts (scikit-learn, 2019). Both models consider a noise (alpha) or smoothing parameter which defines how tightly the response surface fits to the data. Specifically, the RBF is an interpolator only when the smoothing parameter is set to zero, i.e., the RSM passes (exactly) through the evaluated data. However, it is likely that reducing the accuracy of the surrogate at the sample points may improve the overall accuracy.

![Figure 9: Cross-validation study of target surrogate models using a 25% holdout with replications per condition.](image-url)
The accuracy of the selected surrogate models can be assessed using the cross-validation feature in the Nodeworks-RSM. When the cross-validation is set above zero, that percentage of the sample points are held out from the surrogate construction and then the error, i.e., the difference between the actual (full CFD model) response and the surrogate model at the withheld sample location, is calculated and reported in a variety of metrics. To assess the RBF and GP models, the cross-validation is set to 25% and the $L_2$-norm of the withheld sample error is monitored as the smoothing parameters is adjusted over several orders of magnitude. Because the withheld samples are selected randomly, each evaluation is repeated ten times to create an ensemble with a mean of 95% confidence interval (CI). The results of the cross-validation study are presented in Figure 9 which shows a clear sweet spot in all four models considered between smoothing parameter values of $10^{-14}$ and $10^{-6}$. The higher smoothing values of $10^{-8}$ for both the GP model and the RBF model with an epsilon value of unity is selected as the final candidate surrogate models. The candidate surrogate models are statistically similar in accuracy. The GP and RBF models have an $L_2$-norm error from 25% cross-validation of $12.1 \pm 1.4\%$ and $11.9 \pm 2.1\%$.

After narrowing down the surrogate model candidates to two, two final checks are performed. First, Figure 8 seems to suggest that the sample with the highest value of $x_3$ (also with the largest $y_1$ response) appears as a slight outlier in the data. Both models are re-fit, again with ten replicates of 25% cross-validation, excluding this single sample. Neither model shows an improvement in the cross-validation $L_2$-norm error. Therefore, the point is included with the sample. Finally, the cross validation is set to zero so that the two models are fit to the full 64-point sample. Figure 10 provides parity plots of the error relative to the CFD response at the sample points. Again, there is little differentiating the two models. The GP model is taken as the surrogate for optimization. Surface and contour plots of the surrogate in $x_1$-$x_3$ space are shown in Figure 11. In both plots, $x_2$ is held constant at the midpoint.
Figure 11: Visualization of the selected GP surrogate model, 3-D surface at left, contour plot at right, both at mean $x_2$.

The contour plot in Figure 11, an isoline of $y_1 = 2$, can be seen to exist somewhere in between the marked isolines of 1.6 and 2.4. However, this line is only at a fixed value of $x_2$, at the midpoint. In general, a 3-D subsurface characterizing $y_1 = 2$ needs to be extracted from the 4-D surrogate model. The isosurface is extracted from the RSM using Nodeworks’ Optimizer node. Rather than optimizing to an extremum, i.e., the minimum or maximum, the response value is optimized. This is repeated over 1500 times to extract the set of points defining the surface.

An interpolated isosurface of $y_1 = 2$ is displayed in Figure 12; the opensource Octave is used for interpolation and visualization. The surface is colored by the objective function $f = x_3x_2/x_1$. At full scale, the surface is skewed by large values of $f$, particularly at high $x_3$. Therefore, Figure 12 also includes a zoomed in view near the “bottom” of the surface with a significantly reduced $f$ range. This (largely hypothetical) cases seeks to find the single optimal condition.

Figure 12: Isosurface interpolated between values extracted from the GP surrogate model. Surface is colored by objective function $f = x_3x_2/x_1$. 
The optimal operating condition, marked by a black ⊗ symbol on the righthand side in Figure 12, is determined to be: $x_1 = 8.607 \times 10^{-5}$ kg/s, $x_2 = 5.379 \times 10^{-5}$ kg/s, and $x_3 = 4.788 \times 10^{-4}$. The steam to biomass mass flowrate at the optimal condition is: $f = x_3 x_2 / x_1 = 3 \times 10^{-4}$. However, it is worth noting that for a more practical optimization problem it may be desirable to relax the (singular) optimal condition. For example, allowing for some “inefficiency,” i.e., allowing $f$ to increase from the determined optimum of $3 \times 10^{-4}$ to, say $5 \times 10^{-4}$, then a Pareto front of near-optimal operating conditions could be extracted from the $y_1 = 2$ surface in Figure 12 which may allow for more general operating conditions that are not tied to a single flow condition.

### 3.5 SIMULATION OF OPTIMAL OPERATING CONDITION

Finally, the optimal operating condition (which was computed on the surrogate model) is tested with a full, CFD model evaluation. The optimal values are entered as model inputs and a final simulation is run. The composition of the syngas at the reactor outlet (mole fraction) is displayed in Figure 13. The snapshots of gaseous syngas species compositions at 30 s are shown in Figure 14. Averaging the fraction of $\text{H}_2/\text{CO}$ from 25 to 30 s gives a value of $y_1 = 2.205$. The error in the target operating condition ($2.205/2 - 1 \approx 10\%$) is within the expected surrogate model accuracy determined from the cross-validation analysis. The surrogate model discrepancy could potentially be improved by additional samples, however, the underlying CFD predictions may not even be within 10% of the actual values.

![Figure 13: Simulated outlet composition of the syngas at the optimal operating condition determined by the surrogate model.](image-url)
Figure 14: Snapshots of gaseous syngas species mass fraction compositions at 30 s.
4. **CONCLUSIONS**

This work employs MFiX-TFM to model a bench-scale 3-D fluidized bed biomass gasifier. In the simulation, the fluidizing air, the bed material of sand and the biomass particles are all simulated with TFM. The drying, devolatilization, char combustion and gasification, and the homogeneous gaseous reactions are all captured. The outcome syngas composition from the outlet are averaged at steady state. Furthermore, 3 operation conditions including the mass flowrate of the biomass feedstock, the mass flowrate of the fluidizing gas and the mass fraction of steam in the inlet gas are optimized with Nodeworks-OT to reach a hypothetical target of producing a syngas with twice the mole fraction of hydrogen than carbon monoxide, i.e., $\frac{H_2}{CO} = 2.0$. From the results, it is clear that MFiX-TFM is an effective model in predicting the flow behavior and the chemical reactions in a fluidized bed biomass gasifier, and Nodeworks-OT is a useful tool in optimizing the operation conditions to reach the targeted goal.
5. REFERENCES


