Advanced Design Optimization of Combustion Equipment Using Sculptor® with CFD Tools

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Abstract:
Traditional optimization studies on computational fluid dynamic (CFD) models entail changes in geometry and consequent regeneration of computational grids. Depending on the extent of spatial discretization, these changes may be computationally intensive and prove redundant in a computational time frame. SCULPTOR® from Optimal Solutions Software has provided arbitrary shape deformation (ASD) tools that allow 3D shape deformation (i.e. morphing without the need of CAD parameters and without remeshing) of the computational mesh as a result of detailed changes in geometry, allowing efficient, detailed, optimized analysis of CFD models. The case at hand is an extension of advanced burner optimization performed on the standard burner engineering laboratory design, where SCULPTOR was effectively utilized to optimize flame stability for biomass gasification (Smith and Landon, 2013). Further to a base design, this study investigates the effect of changing the annular location of secondary air inlets peripheral to the primary air inlet in a biomass gasifier, as also a change in the diameter of secondary air inlets; affecting swirl, and analyzes the resulting change in flame temperature, recirculation zones and gas phase flow instabilities. From the five cases studied, it was observed that the two secondary locus change cases and the geometry change to the combustor produced estimates (especially for outlet major species mole fractions) very close to the experimental results furnished by Kobayashi et al. (2009).

Introduction and Background:
Ecological protection and emission reduction have brought targeting exit species concentrations from combustion units to the forefront of combustion/gasification design goals. Biomass is bio-degradable, eco-friendly and provides satisfactory energy supply for small-scale applications, where power from coal combustion plants is not necessarily required. However, due to more vastly varying compositions in biomass feedstock as compared to coal, a comprehensive benchmark database is yet to be established and verified.

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In order to target a certain NOx, CO or greenhouse gas exit concentration, an in-depth understanding of physical geometries that influence the initiation and progress of respective solid phase and gas phase reactions is pivotal to the design of a gasification chamber. Investigation of chamber designs in CFD models has generally involved regeneration of meshes with changing geometries. With SCULPTOR®, recursive mesh generation in gasification models can be circumvented (Smith and Landon, 2013). Arbitrary shape deformation (ASD) tools modified the existing geometry, morphing the existing mesh with significant detail at primary and secondary air inlets (341444 mixed cells with over 95% hexahedral) while maintaining cell quality.

**Physical Model Description:**

The base design for biomass gasification is an air-blown entrained-flow type gasifier of lab scale used for experimental studies by Kobayashi et al. (2009), shown in Figure 1. The primary air inlet entrains biomass particles, located concentric to the axis of symmetry. The four secondary air inlets are centered on a concentric locus, intermediate to the primary air inlet and the burner wall.

![Figure 1 - Front and side views of biomass gasification geometry – base case](image)

The generated mesh has 341444 mixed cells composed of HEX cells, TET cells and PRISM cells. The mesh used in the base case was composed of over 95% hexahedral cells as shown in Figure 2. This mesh illustrates the detailed mesh used at the reactor face where primary inlets are located.

**Computational Model Setup and Boundary Conditions:**

Discrete phase model (DPM) was used to model continuous and discrete phases, considering the flow is dilute; Lagrange formulation was utilized to approximate particle tracks coupled with heat and mass transfer resulting from particle motion (Shi et al., 2006). Accordingly, an Euler-Lagrange description of the flow is necessary; an Eulerian formulation by solving conservation equations for mass, momentum and energy for the bulk phase (Versteeg and Malalasekara, 2007) and the Lagrangian formulation for the particle phase.
For a spherical particle, the drag force is defined as (Haberman and Sayre, 1958):

\[ F_D = \frac{18\mu g \text{Re} C_D}{\rho_p d_p^2} \frac{24}{R^2} \]

Eq. 1

The drag coefficient is determined from the Schiller and Naumann (1935) model correlation as:

\[ C_D = \begin{cases} 24(1 + 0.15Re^{0.687})/Re & \text{Re} \leq 1000 \\ 0.44 & \text{Re} > 1000 \end{cases} \]

Eq. 2

Ranz and Marshall’s (1952) Nusselt number correlation is then used to determine the convective heat transfer coefficient:
The standard $k-\varepsilon$ turbulence model was used to model flow phenomena – primarily, eddy dissipation. The SIMPLE scheme was used for pressure-velocity coupling with the least squares technique for the spatial discretization gradient. A second-order spatial discretization upwind scheme was used for momentum, turbulence, energy, species and radiation.

The woody biomass particles are heated till the vaporization/devolatilization temperature is reached. There is no mass transfer or chemical reactions during this stage. When the biomass particles reach a certain temperature, say the vaporization temperature, moisture is released. The chemical reactions and associated kinetics for solid and gas phases are seen to follow: passive heating, devolatilization, volatiles oxidation, char combustion and gasification.

The kinetic devolatilization rate is determined from the Kobayashi et al. (1976) model with two competing rates. The overall weight loss is determined by:

$$\frac{dmv}{dt} = (m_{p,0} - m_a)(\alpha_1 R_1 + \alpha_2 R_2)\exp\left(- \int_0^t (R_1 + R_2)dt\right)$$

where $R_1 = A_1 \exp(-E_1/RT_p)$ and $R_2 = A_2 \exp(-E_2/RT_p)$ are the two competing rates that control the devolatilization over different temperature ranges. The yield factors $\alpha_1$ and $\alpha_2$ represent devolatilization at low and high temperatures, respectively. The yield factors are feed specific and is determined from proximate analysis.

Volatiles Oxidation, Char Combustion and Gasification: After all the volatiles have been released, oxidation of volatiles, char combustion and gasification takes place until all the char is consumed or the particles flow out of the reactor. The chemical reactions include volatile oxidation (combustion), char combustion (oxidation), char-steam gasification, char-carbon dioxide gasification and char-hydrogen gasification, followed by the gas phase reactions.

Volatiles oxidation/combustion for oxygen-rich conditions is given by:

$$C_{m_{11}}H_{m_{12}}O_{m_{13}}N_{m_{14}}S_{m_{15}} + \left(m_{11} + \frac{m_{12}}{4} - \frac{m_{13}}{2} + m_{15}\right) \cdot O_2 \rightarrow C_{m_{11}}O_{2} + \frac{m_{12}}{2} \cdot H_2O + \frac{m_{14}}{2} \cdot N_2 + m_{15} \cdot SO_2$$

Using the expression for the partial oxidation of volatiles from Chen et al (2000), we get the following equation for volatiles oxidation/combustion under oxygen-lean conditions, $\left(\varphi < \left(m_{11} + \frac{m_{12}}{4} - \frac{m_{13}}{2} + m_{15}\right)\right)$:

$$C_{m_{11}}H_{m_{12}}O_{m_{13}}N_{m_{14}}S_{m_{15}} + \varphi \cdot O_2 \rightarrow C_{m_{11}} \cdot (\alpha_1 CO_2 + \alpha_2 CO) + \left(\frac{1-a_1}{2} (m_{12} - 2 \cdot m_{15})\right) \cdot H_2 + \frac{\alpha_1}{2} (m_{12} - 2 \cdot m_{15}) \cdot H_2O + \frac{m_{14}}{2} \cdot N_2 + m_{15} \cdot H_2S$$

$$Nu = \frac{h_d}{k_{\infty}} = 2.0 + 0.6Re_d^{1/2}Pr^{1/3}$$  \hspace{1cm} Eq. 3
Carbon monoxide and hydrogen are produced during the gasification of char particles. The performance of a gasifier is determined primarily by the char gasification reactions. The following particle surface reactions have been included in the model:

\[ C + \frac{1}{2} O_2 \xrightarrow{k3} CO \]  
\[ Eq. 7 \]

\[ C + H_2O \xrightarrow{k4} CO + H_2 \]  
\[ Eq. 8 \]

\[ C + CO_2 \xrightarrow{k5} 2CO \]  
\[ Eq. 9 \]

\[ C + 2H_2 \xrightarrow{k6} CH_4 \]  
\[ Eq. 10 \]

The continuous phase is modeled by using global reactions to describe gas phase chemistry. A set of global reduced reaction kinetics appropriate for gasification studies has been used in the present analysis. The following reaction paths have been considered for this model:

\[ CH_4 + \frac{1}{2} O_2 \xrightarrow{k7} CO + 2H_2 \]  
\[ Eq. 11 \]

\[ H_2 + \frac{1}{2} O_2 \xrightarrow{k8} H_2O \]  
\[ Eq. 12 \]

\[ CO + \frac{1}{2} O_2 \xrightarrow{k9} CO_2 \]  
\[ Eq. 13 \]

\[ CO + H_2O \xrightarrow{k10} CO_2 + H_2 \]  
\[ Eq. 14 \]

A reduced global reactions scheme has been used to lessen the computational burden required when using a detailed reaction mechanism with the eddy dissipation concept. The chemical kinetics of Wu et al. (2010) was employed with some minor changes as shown in Table 1.

**Table 1 - The chemical kinetics parameters used for the competing finite-rate/eddy dissipation model**

<table>
<thead>
<tr>
<th>Reaction Rate</th>
<th>( A ) (s(^{-1}))</th>
<th>( E ) (kJ/kmol)</th>
<th>( n_r )</th>
<th>( \prod_j ) [( C_j )](^{(q_{jr} + q_{jr}^p)} )</th>
<th>A</th>
<th>B</th>
<th>Source</th>
</tr>
</thead>
<tbody>
<tr>
<td>(k1)</td>
<td>2.119 x 10(^{11})</td>
<td>2.027 x 10(^8)</td>
<td>0</td>
<td>[Vol](^{1.2}[O_2]^{1.3})</td>
<td>100</td>
<td>25</td>
<td>FLUENT (2013)</td>
</tr>
<tr>
<td>(k2)</td>
<td>4.4 x 10(^{11})</td>
<td>1.25 x 10(^8)</td>
<td>0</td>
<td>[Vol](^{1.2}[O_2]^{1.3})</td>
<td>100</td>
<td>25</td>
<td>Jones &amp; Lindstedt (1988)</td>
</tr>
<tr>
<td>(k3)</td>
<td>0.052</td>
<td>6.1 x 10(^5)</td>
<td>0</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>Chen et al. (2000)</td>
</tr>
<tr>
<td>(k4)</td>
<td>0.0782</td>
<td>1.15 x 10(^8)</td>
<td>0</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>Chen et al. (2000)</td>
</tr>
<tr>
<td>(k5)</td>
<td>0.0732</td>
<td>1.125 x 10(^8)</td>
<td>0</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>Chen et al. (2000)</td>
</tr>
<tr>
<td>(k6)</td>
<td>1.2 x 10(^{5})</td>
<td>7.53 x 10(^7)</td>
<td>0</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>Govind and Shah (1984)</td>
</tr>
<tr>
<td>(k7)</td>
<td>4.4 x 10(^{11})</td>
<td>1.25 x 10(^8)</td>
<td>0</td>
<td>[CH(_4)](^{0.5}[O_2]^{1.25})</td>
<td>11.5</td>
<td>2.75</td>
<td>Jones and Lindstedt (1988)</td>
</tr>
<tr>
<td>(k8)</td>
<td>2.5 x 10(^{16})</td>
<td>1.68 x 10(^9)</td>
<td>-1</td>
<td>[H(_2)](^{0.3}[O_2]^{1.25}[H_2O]^{-1})</td>
<td>3.1</td>
<td>0.75</td>
<td>Jones and Lindstedt (1988)</td>
</tr>
<tr>
<td>(k9)</td>
<td>3.16 x 10(^{12})</td>
<td>1.67 x 10(^8)</td>
<td>0</td>
<td>[CO](^{1.1}[O_2]^{2.25})</td>
<td>2.1</td>
<td>0.53</td>
<td>Wu et al. (2010)</td>
</tr>
<tr>
<td>(k10f)</td>
<td>5 x 10(^{12})</td>
<td>2.83 x 10(^8)</td>
<td>0</td>
<td>[CO](^{1.5}[H_2O]^{1})</td>
<td>4</td>
<td>0.5</td>
<td>Callaghan (2006)</td>
</tr>
<tr>
<td>(k10b)</td>
<td>9.5 x 10(^{12})</td>
<td>2.39 x 10(^8)</td>
<td>0</td>
<td>[CO](^{1.1}[H_2]^{0.5})</td>
<td>4</td>
<td>0.5</td>
<td>Callaghan (2006)</td>
</tr>
</tbody>
</table>
The proximate and ultimate analysis of this biomass is as shown in Table 2. The chemical composition of the volatiles released from the pulverized wood (biomass) can be estimated by calculations, and a pseudo-compound representing the volatiles can be created for the CFD model in ANSYS Fluent 14.5.

### Table 2 - Proximate and ultimate analysis for the pulverized wood used as feed

<table>
<thead>
<tr>
<th>Proximate analysis (wt %)</th>
<th>Moisture</th>
<th>5.06</th>
</tr>
</thead>
<tbody>
<tr>
<td>Volatile matter</td>
<td>82.95</td>
<td></td>
</tr>
<tr>
<td>Fixed carbon</td>
<td>16.15</td>
<td></td>
</tr>
<tr>
<td>Ash</td>
<td>0.90</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Ultimate analysis (wt %)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Carbon</td>
</tr>
<tr>
<td>Hydrogen</td>
</tr>
<tr>
<td>Oxygen</td>
</tr>
<tr>
<td>Nitrogen</td>
</tr>
<tr>
<td>Sulfur</td>
</tr>
<tr>
<td>Low heating value (MJ/kg)</td>
</tr>
</tbody>
</table>

A Rosin-Rammler size distribution has been used for the pulverized wood particle size. From Kobayashi et al. (2009), the parameters determined for the particle size distribution are as shown in Table 3.

### Table 3 - Rosin-Rammler particle size parameters for the pulverized wood feed

<table>
<thead>
<tr>
<th>Rosin-Rammler parameters</th>
<th>Minimum diameter (mm)</th>
<th>0.05</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Maximum diameter (mm)</td>
<td>0.25</td>
</tr>
<tr>
<td></td>
<td>Mean diameter (mm)</td>
<td>0.10</td>
</tr>
<tr>
<td></td>
<td>Spread parameter</td>
<td>2.5</td>
</tr>
<tr>
<td></td>
<td>Number of diameters</td>
<td>12</td>
</tr>
</tbody>
</table>

There were 12 discrete particle sizes selected for the Rosin-Rammler size distribution with 20 stochastic tries (with random eddy lifetimes) for each diameter to simulate the effect of turbulent dispersion on the pulverized wood particle parcels.

The feeding rate of the pulverized wood is either 19 kg/hr or 27 kg/hr for the four cases considered in this study. Methane gas was supplied from the ignition burner to maintain the gasification temperature due to limitations with the biomass feeder. The injected methane rate was held constant at 1.8 \( m_\text{CH}_4/\text{hr} \) for all cases. The operating conditions used in Kobayashi et al. (2009) were used for this study. The oxygen-carbon molar ratio \((O/C)\) is defined as the input oxygen carbon ratio as defined by the relation:

\[
O/C = \frac{V_{O_2}/22.4 \times 2 + C_OW_{R,O}/16}{C_CW_{R,C}/12 + V_{CH}_4/22.4}
\]

Eq. 15

Where, \( V_{O_2} \) is the amount of injected oxygen \([m_\text{N}_2/\text{hr}]\), \( W_{R,O} \) is the amount of oxygen in the pulverized wood \([\text{kg/ hr}]\), \( V_{CH}_4 \) is the amount of preheating methane \([m_\text{N}_2/\text{hr}]\) and \( W_{R,C} \) is the amount of carbon in the pulverized wood \([\text{kg/ hr}]\). Biomass was fed at a steady mass flow rate of 19 kg/hr with an O/C ratio of 1.83.
The parameters for the competing-rate (Kobayashi et al., 1976) devolatilization model were taken from Payette and Tillman (2001) for woody biomass as shown in Table 4. The temperature at which the devolatilization begins for the pulverized wood particles was taken to be 506.15K.

Table 4- The Kobayashi devolatilization model parameters used for pulverized wood

<table>
<thead>
<tr>
<th>Devolatilization parameters</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>$A_1$ (s⁻¹)</td>
<td>1.17</td>
</tr>
<tr>
<td>$E_1$ (J/kmol)</td>
<td>$2.851 \times 10^6$</td>
</tr>
<tr>
<td>$A_2$ (s⁻¹)</td>
<td>5.74</td>
</tr>
<tr>
<td>$E_2$ (J/kmol)</td>
<td>$1.432 \times 10^7$</td>
</tr>
<tr>
<td>$\alpha_1$</td>
<td>0.79</td>
</tr>
<tr>
<td>$\alpha_2$</td>
<td>0.98</td>
</tr>
</tbody>
</table>

The temperature boundary conditions for the biomass gasifier are as shown in Table 5.

Table 5 - The temperature boundary conditions used in the model

<table>
<thead>
<tr>
<th>Boundary name</th>
<th>T (K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Biomass inlet</td>
<td>700</td>
</tr>
<tr>
<td>Air inlet</td>
<td>850</td>
</tr>
<tr>
<td>Wall</td>
<td>1040</td>
</tr>
</tbody>
</table>

The turbulence intensity was set at 8% for the biomass inlet and at 10% for the air inlet specifying the hydraulic diameters for these inlets, with use of the standard k-ε turbulence model. The weighted sum of grey gases model (WSGGM) was used along with the discrete ordinates model for radiation. The particle scattering factor is 0.3 and emissivity 0.5. The wall internal emissivity was selected as 0.16

Optimization Study Using SCULPTOR® Based Design Framework:

Optimal Solutions Software, LLC, (OSS) has developed a novel methodology called Arbitrary Shape Deformation (ASD) that helps solve critical problems in computer aided engineering (CAE) design:

- Inadequate shape parameterization algorithms.
- Inadequate algorithms for CAE (CFD and FEA) grid shape modification.

Traditional CAD parameters often fail to provide the correct parameterization required to accurately capture the governing physics involved in shape optimization. ASD enables an engineer to control and manipulate the shape of any geometry from CAD/CAM data or CFD/FEA computational grids. To use ASD, one defines a set of control points around the object to be deformed. These control points are then moved and the underlying functions morph the entity into a new shape. This approach allows the user to mold the shape as if they were a sculptor molding clay. This concept can be illustrated using a physical analogy.
Consider a volume of clear, flexible plastic, in which an object to be deformed has been embedded. The embedded object has the same degree of flexibility as the volume so that as the plastic volume is deformed, the embedded object is also deformed accordingly (see Figure 3 and Figure 4). The volume is modeled as a tri-variate parametric volume with its deformation controlled by a small set of control points. In creating the ASD, the user controls the number of control points used as well as where each control point is located. The ASD technology and the accompanying graphical user interface tools to create and visualize the shape deformation process are part of OSS’ commercial software, SCULPTOR®.

Figure 3- A spherical ball (mesh) is embedded in an ASD grid. Control points are moved and the ASD grid is deformed, causing the ball (the mesh) to deform.

Figure 4- ASD volumes created around Formula Race car front wing. Parametrically rectangular ASD volume used to examine wing shape changes with real-time smoothed deformation of middle wings’ sections angle of attack to show smooth transition between morphed and non-morphed locations.

SCULPTOR® BACKGROUND

ASD solves the first problem listed above by allowing the design engineer to freely create unique shape parameters instead of being restricted to the parameters found in the CAD model. The second problem is solved as SCULPTOR® performs a smooth volumetric deformation in real-time without having to redo the CAD model. Both of these features eliminates the high cost of remeshing for each unique shape.
considered. SCULPTOR® can perform a design change in seconds which normally requires hours (or days) to complete if one has to redo the CAD model for the new shape and then remesh this in the CFD model. SCULPTOR® also allows the design engineer to parameterize, deform and optimize shapes into new and improved designs by providing automated shape and mesh changes.

SCULPTOR® has been applied to design optimization for internal and/or external flow problems in the aerospace, automotive, chemical processing, biomedical, electronics, power generation, turbo machinery, and marine industries. This tool can be applied to any problem where the shape affects the system performance through the associated physics (i.e., fluid flow, heat/mass transfer, chemical reactions, combustion, structural mechanics, fluid structure interaction, etc.) The following list summarizes SCULPTOR® capabilities:

1. Import and export any CAE model (CFD and/or FEA) and/or CAD files with commercial (and in-house codes) including Fluent, StarCD, StarCCM+, ICEM-CFD, Plot3D, Nastran, Ansys, Abaqus, Fieldview, CRUNCH, STL, IGES, STEP, and many other file formats,
2. Innovative advanced tools in a Graphical User Interface that is easy to learn and use to create the ASD volumes for any shape including irregular shapes and topologies,
3. Create user-defined shape change parameters with control points grouped together into shape change variables where each control point is defined to move in its own directions allowing shape changes to be defined in terms of translate, rotate, or scale the geometry or mesh shape,
4. Maintain fine local control of deformation for subtle shape changes since the best shape change to improve performance may be small and subtle, thus requiring the need for highly accurate smooth shape deformations,
5. Large deformation capabilities for useful conceptual design exploration,
6. Maintain high mesh quality for viscous surface mesh thickness and shape,
7. Perform rigid body deformations of components within the flow domain mesh (for problems such as wing flap rotation, valve movement, etc.),
8. Perform deformation in real-time without the need to revisit CAD or remesh,
9. Calculate and monitor the computational mesh quality in real-time during the deformation process and use the mesh quality measurements as constraints in the optimization process,
10. Deform multiple CFD and/or FEA grids simultaneously,
11. Optimize with a built-in Gradient-based Optimization Algorithm (GRG – Generalized Reduced Gradient) or Design of Experiments with Optimal Latin Hypercube and Response Surface Methodology,
12. Use in batch-mode execution with external optimization tools including Simulia iSIGHT, ModeFrontier, Phoenix Integration, Opitmus, DAKOTA, Matlab and others, and
13. Sending optimized shape back to CAD by applying the optimal shape deformation to the CAD model via IGES, STEP, ACIS, ParaSolids file formats so the user can interactively deform a CAD model directly using SCULPTOR®.

SCULPTOR® has been used worldwide by design engineers in many industries including aerospace, aircraft, marine, turbo machinery, biomedical, fossil energy, oil and gas, petroleum and others.
CURRENT SCULPTOR® APPLICATION

The parameters for the current analysis included CO, CO2, H2O mole fractions and temperature profiles in the devolatilization and gasification zones and at the gasifier outlet plane (see Table 6):

Table 6- Design parameters for Biomass Gasifier Optimization

<table>
<thead>
<tr>
<th>Design Parameter</th>
<th>Original Dimension (mm)</th>
<th>New Dimension (mm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Diameter of locus of secondary air inlet centers</td>
<td>180</td>
<td>170</td>
</tr>
<tr>
<td>Diameter of locus of secondary air inlet centers</td>
<td>180</td>
<td>190</td>
</tr>
<tr>
<td>Secondary air inlet diameter</td>
<td>50</td>
<td>40</td>
</tr>
<tr>
<td>Diameter of cross-section 300 mm downstream of air inlets</td>
<td>255</td>
<td>280</td>
</tr>
</tbody>
</table>

Accordingly, the ASD tool was used to remesh at geometric zones selected for shape deformation. The number of cells in all meshes was maintained constant but re-ordered as shown in Figure 3 (a) – (d). This process shows that it is possible to deform loci of uniform geometric shapes (locus of diameter of secondary air inlets), as also smooth deformation into non-uniform regions with retention of mesh continuity and alignment over deformed interfaces (cross-section deformation over 300 mm downstream from inlet cross section).

![Figure 5- Meshes for (a) diameter of locus of secondary inlet centers at 170 mm, (b) diameter of locus of secondary inlet centers at 190 mm, (c) secondary inlet diameter at 40 mm, and (d) ASD of region 300 mm downstream from inlet cross section](image-url)
Results and Discussion:

Computing resources at the Energy Research and Development Center (ERDC) at Missouri University at Science and Technology, Rolla (MO) were utilized for this purpose. This consisted of two Intel Xeon X-5690 CPUs (2 x 6 processors) running at 3.46GHz with 48GB RAM. Typically, each run met the convergence criteria within 6 to 8 hours of CPU time when 10 processors were utilized.

The analyses consisted of five different CFD calculations including (a) base case design, (b) secondary separation (locus) changed from 180mm to 170mm, (c) the locus changed from 180mm to 190mm, (d) the secondary diameters changed from 50mm to 40mm, and (e) Inclusion of a convex bulge (bulb) portion near the inlet of the gasifier.

As can be seen, the temperature distributions for all five cases are similar except for Case 4 where the secondary inlet diameter was changed from 50mm to 40mm. For this case, gasification is initiated further upstream compared to the other cases which results in a higher observed peak temperature (1815K) along
the gasifier axis as shown in Figure 6d. In all the other cases, the maximum peak temperature is observed 0.45m to 0.55m downstream of the inlet (with similar flame shapes) with the peak temperature within the gasifier not exceeding 1740K.

As shown in Figure 7, most of the CO release occurs well into the second half of the gasifier, downstream of the char burnout region for all cases considered. The magnitude of both the peak CO concentration as well as the outlet CO concentration is less in Case 4 (see Figure 7d) compared to the other cases. The gasifier outlet CO concentration is nearly the same for Cases 2, 3 and 5, which agrees very well with experimental results of Kobayashi et al. (2009) with an error of less than 3%.

![Figure 7 - CO mole fraction contours for design analysis of biomass gasifier](image)

The highest formation of H2 is predicted to occur around 0.25m to 0.3m downstream of the reactor inlet (see Figure 8). The magnitude of both the peak H2 concentration as well as the H2 concentration at the outlet is less in Case 4 (see Figure 8d) as compared to the other cases. The gasifier outlet H2 concentration
is also very similar for Cases 2, 3 and 5, again quite similar to Kobayashi’s experimental results (see Kobayashi et al. 2009).

(a) Case 1: Base Case Design

(b) Case 2: Secondary locus changed from 180 to 170 mm

(c) Case 3: Secondary locus changed from 180 to 190 mm

(d) Case 4: Secondary diameter changed from 50 to 40 mm

(e) Case 5: Adding convex bulb in gasifier inlet region

Figure 8: H2 mole fraction contours for design analysis of biomass gasifier

The predicted peak CO2 formation is observed immediately downstream of the highest observed H2, again along the gasifier axis (see Figure 9). The magnitude of both the peak CO2 concentration as well as the concentration at the gasifier outlet is less in Case 4 (see Figure 9d) as compared to the other cases considered. The gasifier outlet CO2 concentration is very similar for Cases 2, 3 and 5. However, for the CO2 gasifier outlet concentration, Case 4 predicted concentrations are closest to experimental results (Kobayashi et al. (2009)).
Comparing all results together (see Figure 10) it is seen that the predicted outlet species mole fractions for CO₂, H₂ and CO for the different design cases agree well with the experimental results of Kobayashi et al. (2009). Specifically, the outlet CO concentrations for Cases 2, 3 and 5 are very close to the experimental results of Kobayashi et al (2009) with an error of less than 3%. The same is seen for H₂ concentration while the CO₂ concentration at the gasifier outlet for Case 4 is closest to Kobayashi’s experimental results again with an error of slightly more than 3%.

Overall, it is observed that for Cases 2, 3, and 5), the secondary locus at 170mm, the secondary locus at 190mm and the ASD case agree well with experimental results.
From Figure 11, it can be observed that the temperature distributions are similar for all the cases except Case 4, which includes results for decreasing the secondary inlet diameter from 50mm to 40mm. The temperature in the other four cases does not vary more than 4%, with the maximum difference predicted to occur close to the gasification zone. In this zone, when compared with the experimental data, the difference amounts to an error of less than 4%.
Conclusions:

The gasification model was set up in ANSYS Fluent with the Euler-Lagrange DPM with a competing finite-rate/eddy dissipation sub-model. After the Base Case was successfully completed, SCULPTOR® was used to deform the geometry (Case 5) and reorder the respective mesh for all cases except for Case 1 which enabled a more efficient parameterization study and allowed consideration of using an ASD to perform reactor shape deformation. From this study, it was observed that the temperature distribution was similar for the four design cases except for Case 4 which considered decreasing the secondary air inlet diameter from 50mm to 40mm. Also, it appears there is closer agreement with experimental data for the outlet species mole fractions of CO and H₂ for Cases 2, 3 and 5 while for CO₂, Case 4 appeared to provide the best agreement to experimental data.

References: