CFD Models Applied to Gasification Improvement and Optimization

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Summary

Development of numerical models applied to biomass gasification:

- Biomass gasification: an overview

- Development of a comprehensive 2-D multiphase model to predict syngas composition from waste residues

1.Biomass Gasification

Why Biomass Gasification?

- As a result of environmental and other policy considerations, there is an increasing world-wide interest in the use of biomass resources.

- Biomass gasification technologies are expected to be an important part of the effort to mitigate global climate change by expanding the use of biomass.

- Gasification technologies provide the opportunity to convert biomass feedstock into clean multi-component fuel gas or synthesis gases (syngas).

Using Biomass

What is biomass?

- All organic material that stems from plants, trees and crops and also the non-fossilized and biodegradable material from animals and micro-organisms

Biomass can be obtained from:

- Organic waste streams
- Wood Residues
- Agricultural and forestry residues

Using Biomass

Advantages of using biomass?

- Potential of biomass energy is much larger than the current world energy consumption and is always available
- Reduces the need for fossil fuels for the production of heat and electricity
- Growing biomass crops produce O_2 and use up CO_2

Disadvantages of using biomass:

- Availability of lands for energy plantations can be problematic
- Regeneration problems
- Cost *vs* governmental policy measures

1.2.BiomassConversion Processes

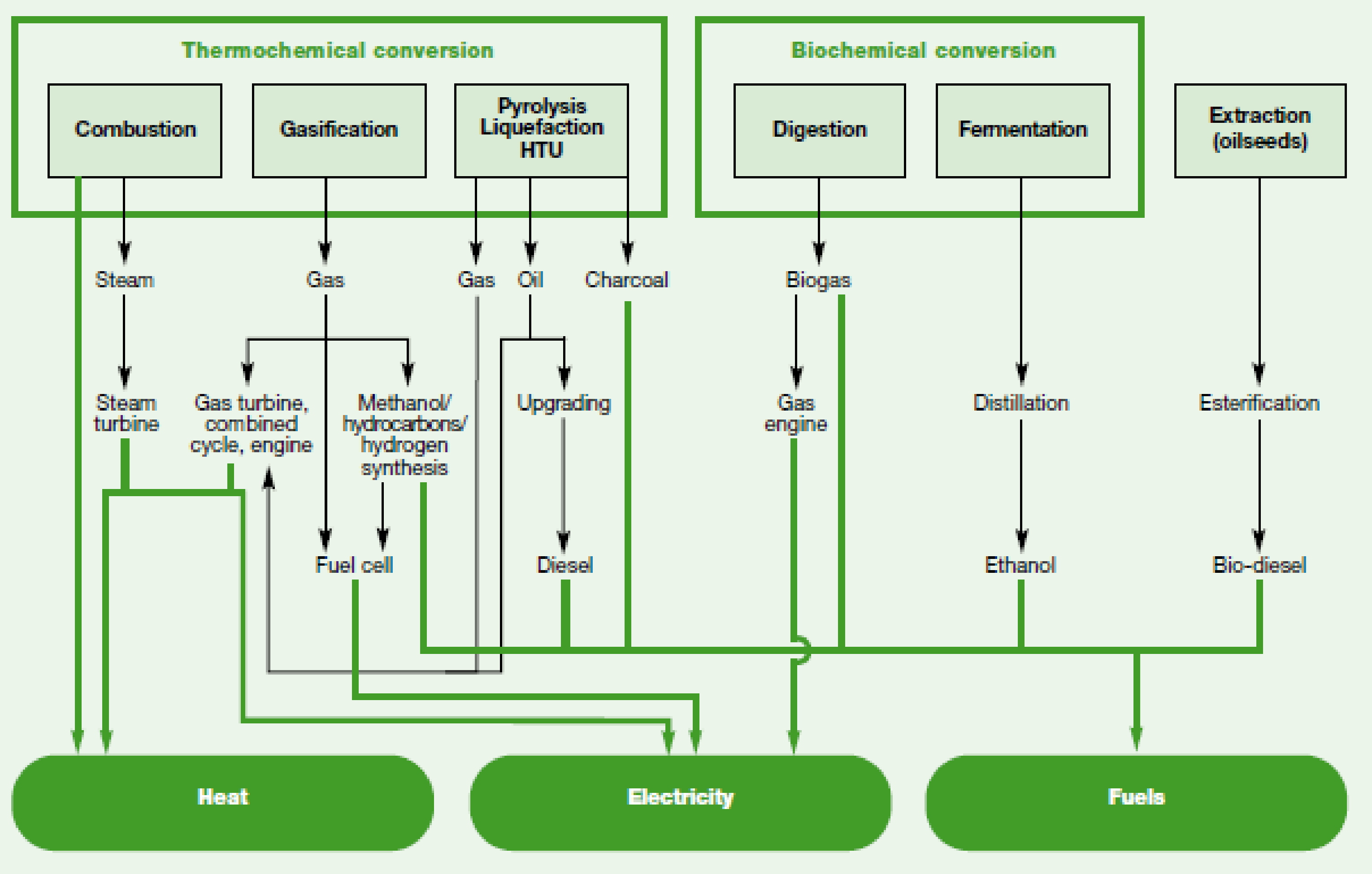
Biomass Conversion

Biomass conversion can be subdivided:

- **Thermochemical processes**
  - Combustion
  - Pyrolysis
  - Gasification

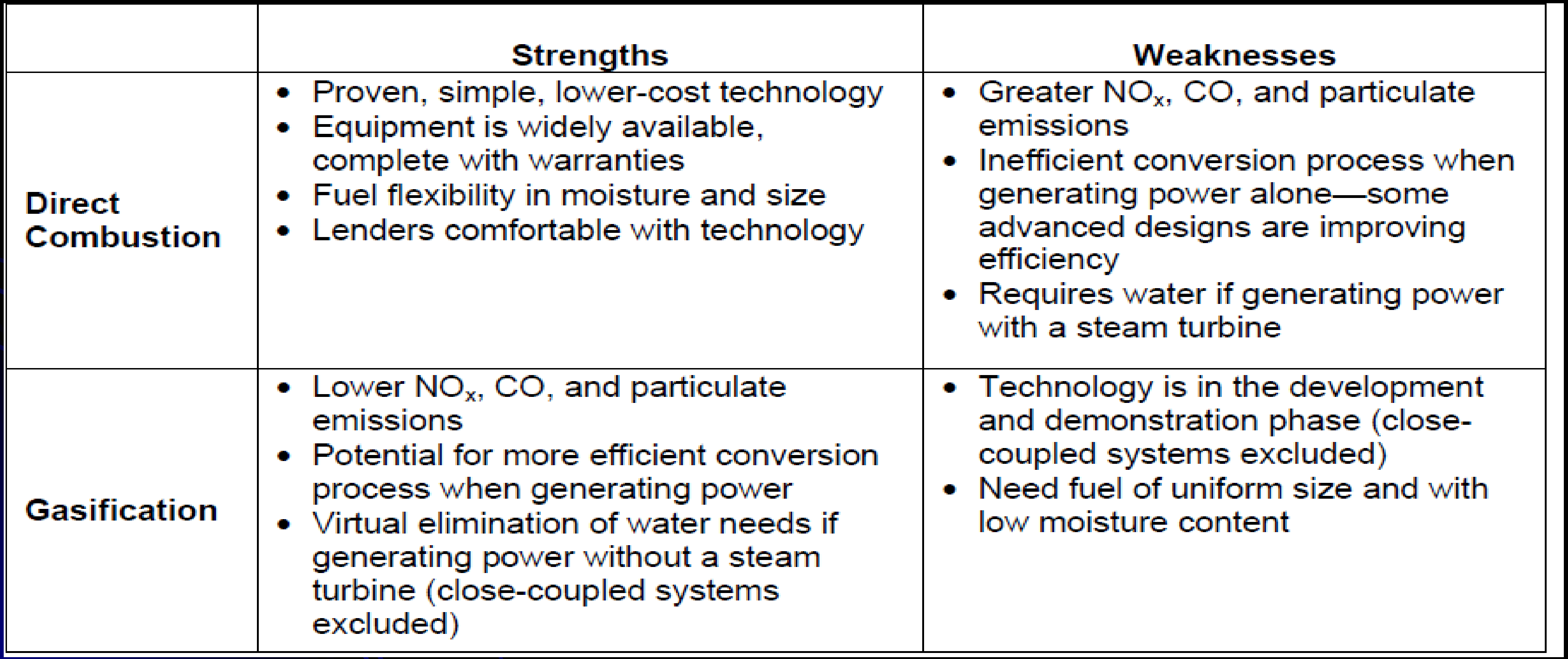
- **Biochemical Processes**
  - Digestion
  - Fermentation

Biomass Conversion



Gasification *vs* Combustion

Strenghts and weakenesses of gasification and combustion:



	Strengths	Weaknesses
Direct Combustion	• Proven, simple, lower-cost technology • Equipment is widely available, complete with warranties • Fuel flexibility in moisture and size • Lenders comfortable with technology	• Greater NO_x, CO, and particulate emissions • Inefficient conversion process when generating power alone—some advanced designs are improving efficiency • Requires water if generating power with a steam turbine
Gasification	• Lower NO_x, CO, and particulate emissions • Potential for more efficient conversion process when generating power • Virtual elimination of water needs if generating power without a steam turbine (close-coupled systems excluded)	• Technology is in the development and demonstration phase (close-coupled systems excluded) • Need fuel of uniform size and with low moisture content

Biomass Gasification

- Incomplete combustion due to the surplus of the solid fuel, resulting in the production of combustible gases as CO, H_2 and traces of CH_4

Producer gas / syngas

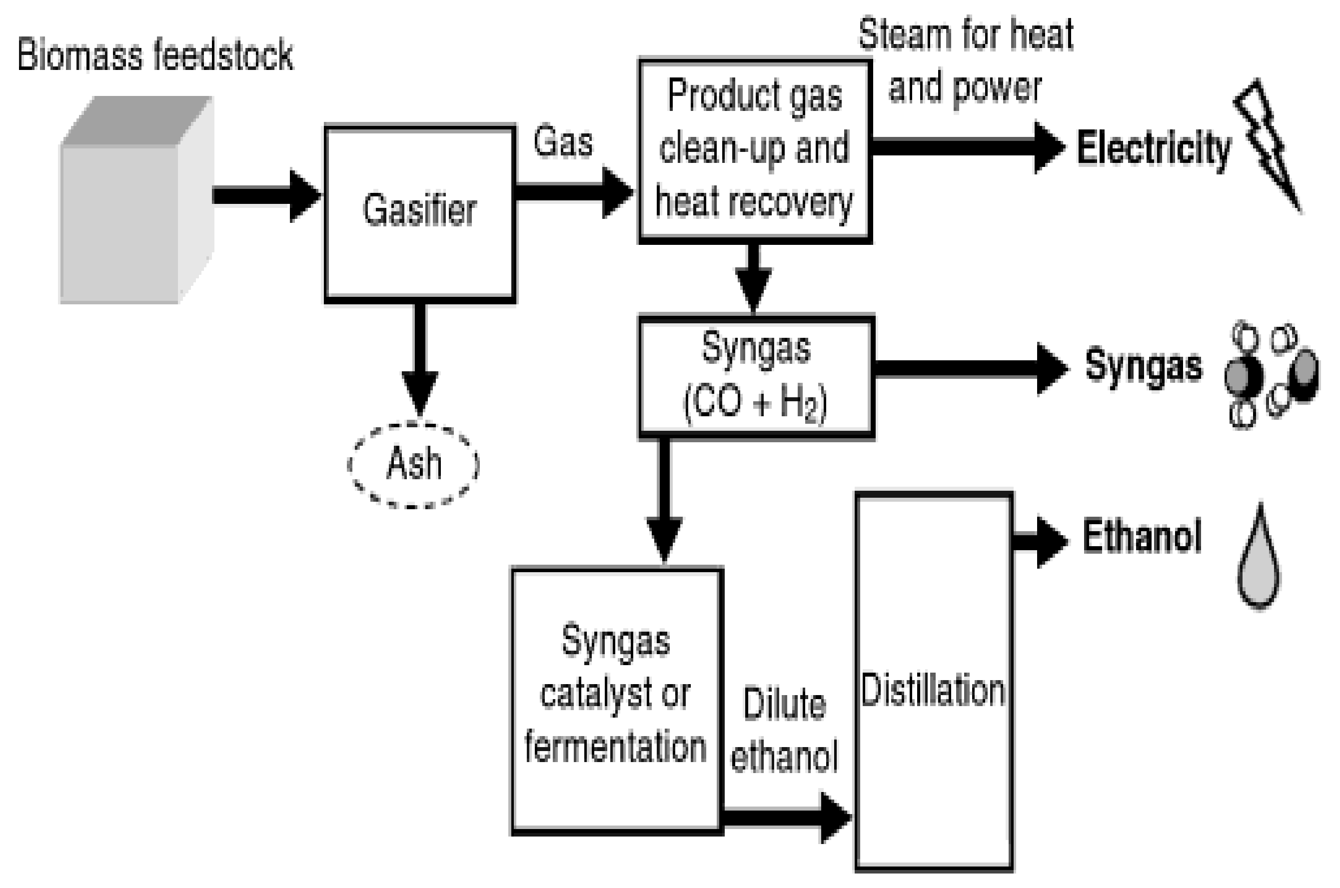
- The producer gas can be used:
  - To be run in internal combustion engines
  - To be applied to fuel cells
  - To heat purposes

Biomass Gasification

- **Products of gasification:**
  - ☐ **Hydrocarbon gases**
  - ☐ **Hydrocarbon liquids (oils)**
  - ☐ **Tars (carbon black and ash)**

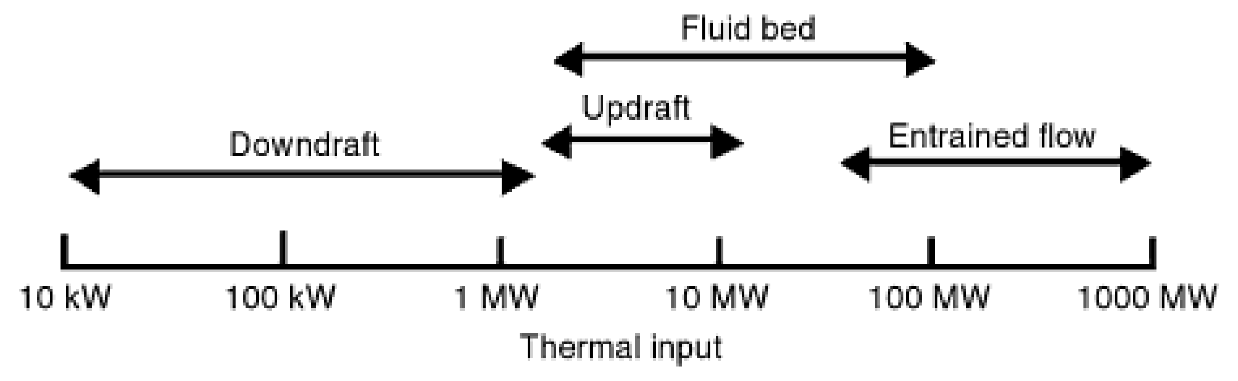
- **Gasification technology challenges:**
  - ☐ **Biomass feedstock quality**
  - ☐ **Reliable experimental data**
  - ☐ **Scale-up**
  - ☐ **Energy efficiency optimization strategies**
  - ☐ **Numerical simulation**

Biomass Gasification



Gasification Reactors

- Gasifier types:
  - ☐ Downdraft
  - ☐ Updraft
  - ☐ Fluidized bed
  - ☐ Entrained flow



Bubbling Fluidized Bedgasifiers

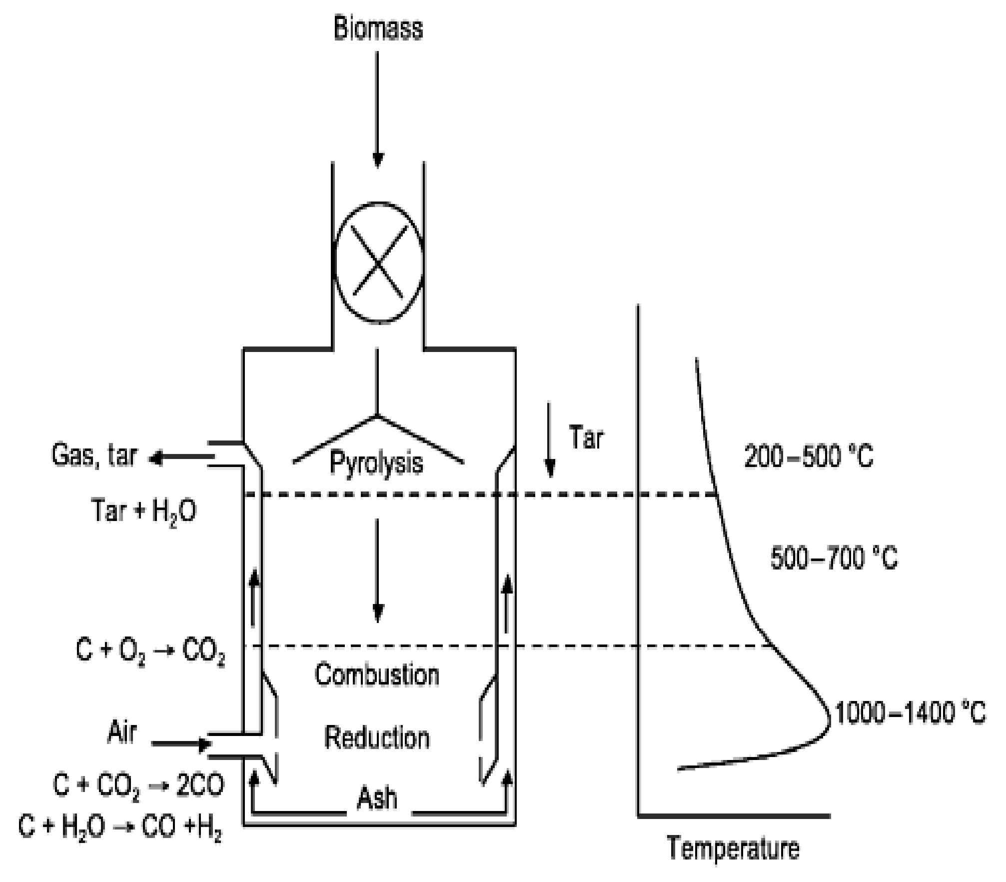
Advantages:

- Yields a uniform syngas
- Nearly uniform temperature distribution
- Able to accept a wide range of fuel particles sizes
- High conversion with low tar and unconverted carbon

Disadvantages:

- Large bubble size may result in gas bypass through the bed

Downdraft Gasifiers



2. CFD Models

Modelling Approaches

Why developing gasification models:

- Gasification is a complex phenomenon
- The gasifier is one of the least-efficient unit operation
- Provides different scenarios without carrying out experimental procedures (time and money consuming)

Biomass gasification models:

- Equilibrium approach: thermodynamic
- Kinetic
- CFD
- Aspen / Ansys

Experimental and Numerical Analysis of Coffee Husks biomass Gasification in a Fluidized bed Reactor

- **To optimize the operating conditions of a biomass gasification process, it was developed a numerical model based on the computational fluid dynamics (CFD) framework.**

- **Two-dimensional computational model that described the biomass gasification process in a fluidized bed reactor using coffee husks.**

- **The experimental data was gather from a pilot thermal gasification plant, installed at Portalegre's Industrial Park based on the fluidized bed technology.**

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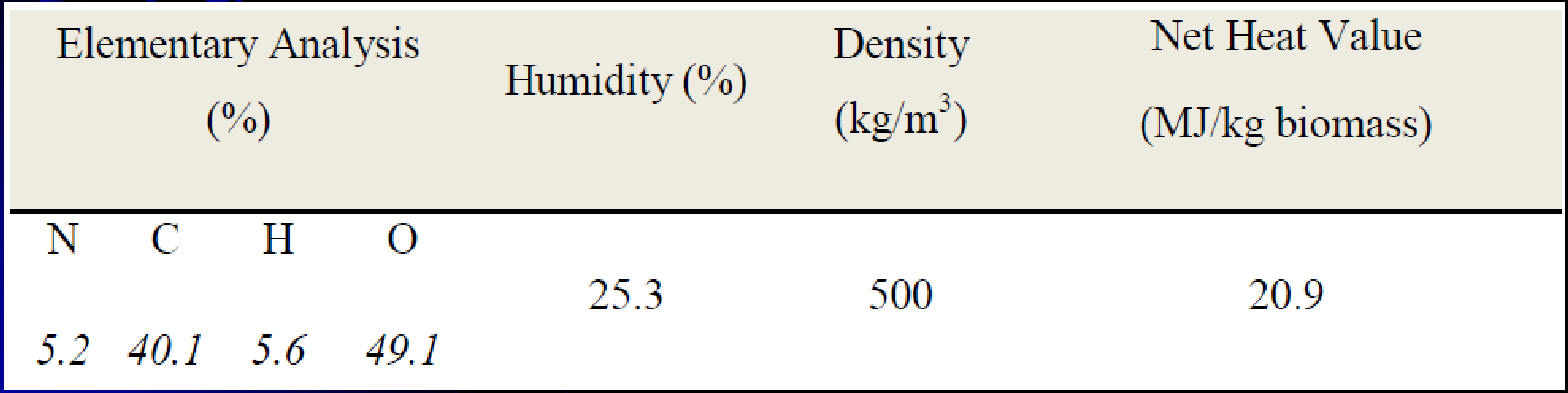

Elementary Analysis (%)				Humidity (%)	Density (kg/m^3)	Net Heat Value (MJ/kg biomass)
N	C	H	O			
5.2	*40.1*	*5.6*	*49.1*	25.3	500	20.9

CFD Numerical Model

- **The model is multi-phase (two phases: gas and solid), where the solid phase is described, given their nature, through an Eulerian Granular model.**

- **Interaction between both phases most be modeled as well, since both phases exchange heat by convection, momentum (given the drag between gas phase and solid phase) and mass (given the heterogeneous chemical reactions).**

- **The chemical model involves 3 heterogeneous and 5 homogeneous chemical reactions**

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Mass Balance

continuity equation for gas phases:

$$\frac{\partial}{\partial t}\left(\alpha_g \rho_g\right) + \nabla \cdot \left(\alpha_g \rho_g v_g\right) = S_{gs}$$

continuity equation for solid phases:

$$\frac{\partial}{\partial t}\left(\alpha_s \rho_s\right) + \nabla \cdot \left(\alpha_s \rho_s v_s\right) = S_{sg}$$

mass source term due to heterogeneous reactions:

$$S_{sg} = -S_{gs} = M_C \sum \gamma_C R_C$$

gas phase density:

$$\frac{1}{\rho_g} = \frac{RT}{p} \sum_{i=1}^{n} \frac{Y_i}{M_i}$$

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Momentum Balance

Momentum equation of gas phase:

$$\frac{\partial}{\partial t}\left(\alpha_g\rho_g v_g\right)+\nabla\cdot\left(\alpha_g\rho_g v_g v_g\right)=-\alpha_g\nabla p_g+\alpha_g\rho_g g+\beta\left(v_g-v_s\right)+\nabla\cdot\alpha_g\tau_g+S_{gs}U_s$$

Momentum equation of solid phase:

$$\frac{\partial}{\partial t}\left(\alpha_s\rho_s v_s\right)+\nabla\cdot\left(\alpha_s\rho_s v_s v_s\right)=-\alpha_s\nabla p_s+\alpha_s\rho_s g+\beta\left(v_g-v_s\right)+\nabla\cdot\alpha_s\tau_s+S_{sg}U_s$$

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Energy Conservation

$$\frac{\partial\left(\alpha_q \rho_q h_q\right)}{\partial\left(t\right)} + \nabla\cdot\left(\alpha_q \rho_q \vec{u}_q h_q\right) = -\alpha_q \frac{\partial\left(p_q\right)}{\partial\left(t\right)} + \bar{\tau}_q : \nabla\left(\vec{u}_q\right)$$

$$- \nabla\cdot\vec{q}_q + S_q + \sum_{p=1}^{n}\left(\vec{Q}_{pq} + \dot{m}_{pq} h_{pq} - \dot{m}_{qp} h_{qp}\right)$$

where:

$$Q_{pq} = h_{pq}\left(T_p - T_q\right)$$

$$h_{pq} = \frac{6 k_p \alpha_q \alpha_p Nu_q}{d_p^2}$$

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Turbulent Model

The standard k-ε model in ANSYS FLUENT

The turbulence kinetic energy, k, and its rate of dissipation, ε, are obtained from the following transport equations:

$$\frac{\partial}{\partial t}(\rho k)+\frac{\partial}{\partial x_i}(\rho k u_i)=\frac{\partial}{\partial x_j}\left[\left(\mu+\frac{\mu_t}{\sigma_k}\right)\right]+G_k+G_b-\rho\varepsilon-Y_M+S_k$$

$$\frac{\partial}{\partial t}(\rho\varepsilon)+\frac{\partial}{\partial x_i}(\rho\varepsilon u_i)=\frac{\partial}{\partial x_j}\left[\left(\mu+\frac{\mu_t}{\sigma_\varepsilon}\right)\frac{\partial\varepsilon}{\partial x_j}\right]+C_{1\varepsilon}\frac{\varepsilon}{k}\left(G_k+C_{3\varepsilon}G_b\right)G_k-C_{2\varepsilon}\rho\frac{\varepsilon^2}{k}+S_\varepsilon$$

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Granular Eulerian Model

- Appropriate for modeling Fluidized beds.
- Normally chosen when more than 11% of content is solid.
- Can calculate granular temperature (solids fluctuating energy) for each solid phase.

The conservation equation for the granular temperature:

$$\frac{3}{2}\left[\frac{\partial\left(\rho_s \alpha_s \theta_s\right)}{\partial t} + \nabla \cdot \left(\rho_s \alpha_s \vec{v}_s \theta_s\right)\right] = \left(-p_s \bar{I} + \bar{\tau}_s\right) : \nabla\left(\vec{v}_s\right) + \nabla \cdot \left(k_{\theta a} \nabla\left(\theta_s\right)\right) - \gamma_{\theta a} + \phi_{ls}$$

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The homogeneous reactions are based in the Eddy Dissipation Model:

Steam Production: $H_2 + \frac{1}{2}O_2 \rightarrow H_2O$

CO Combustion: $CO + \frac{1}{2}O_2 \rightarrow CO_2$

CH_4 Combustion: $CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O$

CH_4 steam reforming reaction: $CH_4 + H_2O \rightarrow CO + 3H_2$

Water-shift Reaction: $CO + H_2O \rightarrow CO_2 + H_2$

Experimental and Numerical Analysis of Coffee Husks biomass Gasification in a Fluidized bed Reactor

Chemical Reactions Model

Heterogeneous reactions

Reduction:	$C + CO_2 \rightarrow 2CO$
Char Combustion:	$C + \frac{1}{2}O_2 \rightarrow CO$
H_2O Char Gasification:	$C + H_2O \rightarrow CO + H_2$

The chemical reactions are based in the kinetic surface diffusion model

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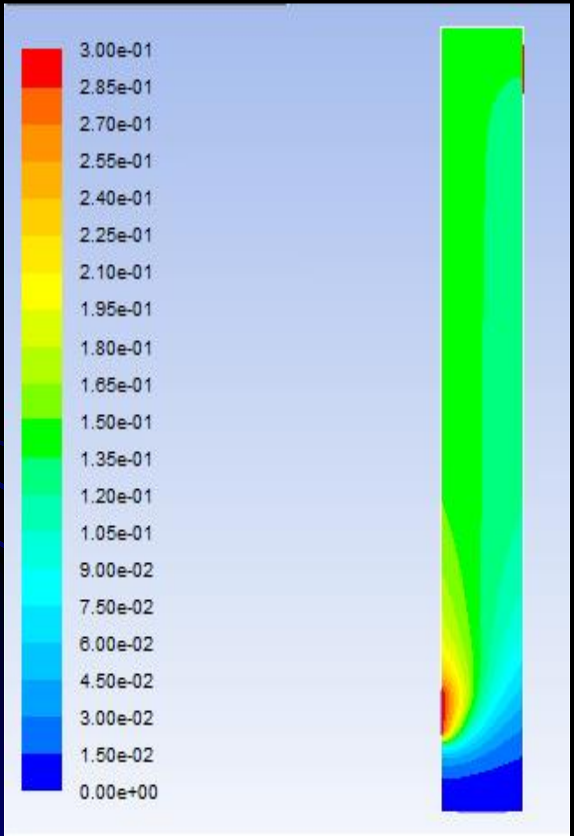

Mass Fraction Contours for CO

Experimental conditions	**Coffee husk**
Temperature (ºC)	815
Admission Biomass (kg/h)	28
Air Flow Rate (Nm^3/h)	75
Ratio $O_2/O_{2\ \text{Stoichiometric}}$	2.63
Syngas fraction (dry basis)	
H_2	12.4
CO	11.4
CH_4	1.6
CO_2	18.7
N_2	52.3

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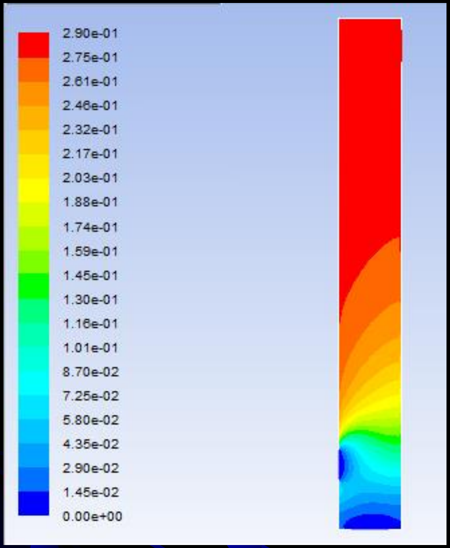
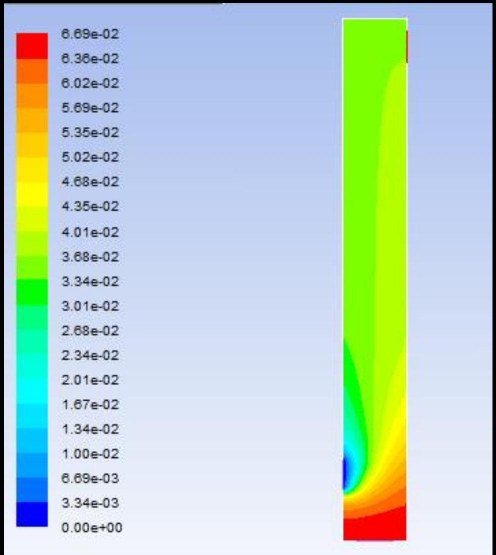


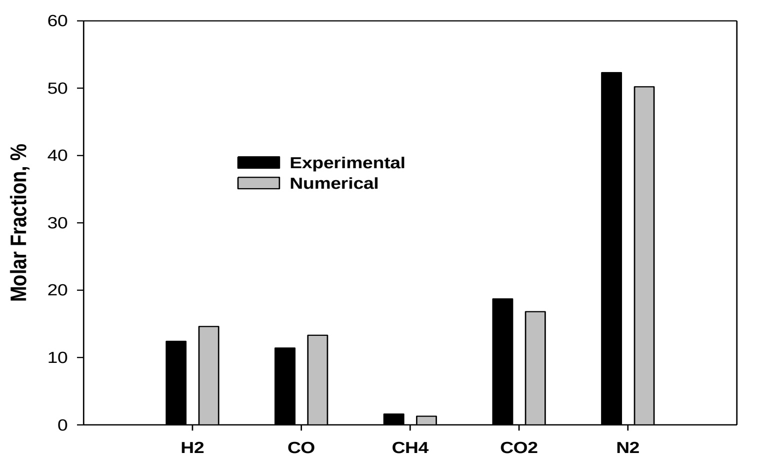
Mass Fraction Contours for CO_2



Mass Contours for H_2O

- ➢The higher values for CO are located immediately above the air in lets, while for CO_2, at a greater height.
- ➢H_2O values are higher near the air inlet and its exit value it obtained immediately above the biomass inlet.

- ➢Measured and computed exhaust gases' composition shows good agreement.
- ➢The major disagreement is found in the concentrations of CO and H_2.



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