THREE-DIMENSIONAL NUMERICAL SIMULATION OF REACTOR AND AXIAL CYCLONE IN SEMI INDUSTRIAL SCALE

Guilherme Maciel[a], Karina Silva[a], Cassius Ferreira[a], Valério Luiz Borges[a], Solidônio Carvalho[a,*], Marcelo Braga dos Santos[a].

[a]Universidade Federal de Uberlândia, Av. João Naves de Ávila, 2121- Santa Mônica, Uberlândia-MG, 38408-100
guilherme.maciel@ufu.br karinadepaula@ufu.br cassiusferreira@ufu.br valerioluizborges@ufu.br, marcelo.bragadossantos@ufu.br solidonio@ufu.br.

ARTICLE INFO

***Keywords**: Ansys, gasification, cyclone, syngas, waste to energy.*

Received: Jan 28, 2024
Reviewed: Feb 07, 2024
Accepted: Mar 15, 2024

ABSTRACT

This study is motivated by the production of synthesis gas (syngas) from gasification of refused-derived fuel (RDF) in thermochemical reactors. For this purpose, a reactor with a circulating fluidized bed transforms RDF into synthesis gas at temperatures around 850°C. The syngas consists of a biphasic mixture, containing fuel gas and solid particles that are dragged during the gasification process. The gas flows into an axial cyclone positioned inside the upper part of the reactor, so that non-gasified particulates, inert residues and particles from the bed can be removed. Due to the size and density of the solid particles and the residence time inside the thermochemical reactor, the cyclone must be designed to clean the gas, improving its quality and reducing costs with scrubbers. Therefore, in this study, a vertical cylindrical reactor with 10.57 m height and 0.95 m diameter was modeled computationally, with an axial cyclone inside measuring 9.3 m in height and 0.6 m in the largest diameter region. The model does not consider thermochemical reactions inside the reactor. For the solid phase, 0.425 m³ of 100 mesh sand particles with a constant density equal to 1500 kg/m³ were considered. For the gas phase an air flow of 800 kg/h at 500°C was adopted. Numerical-computational models were solved using the ANSYS® software, based on the classical equations of mass conservation, momentum and energy. The k-omega SST turbulence model has been applied. From the analysis of pressure gradient, velocity profiles and the particulate removal rate in the cyclone, the cyclone efficiency and the pressure drop were determined. An efficiency of 99.83% in the cleaning process carried out by the axial cyclone was observed. The obtained results also allowed analyze the distribution of particles inside the reactor and their passage in the axial cyclone.

NOMENCLATURE

k	turbulent kinetic energy, J/kg
u, v, w	velocity components, m/s
x,y,z	cartesian coordinates, m

Greek symbols

α,β	turbulent coefficients, dimensionless
υ	dynamic viscosity, Pa s
ρ	density, kg/m^3
σ	Prandtl coefficient, dimensionless
ω	specific rate of dissipation, 1/s

1. INTRODUCTION

The management of municipal solid waste (MSW) is a problem concerning government across the world, since its production is inevitable, hence it is imperative to seek sustainable routes to its disposal. An interesting alternative to solve this problem is the gasification process, which consists of converting MSW in various gaseous components at a high temperature generating the so-called synthesis gas (syngas), which is a flammable gas that can be

* Corresponding author: Solidônio Carvalho. Universidade Federal de Uberlândia, Av. João Naves de Ávila, 2121- Santa Mônica, Uberlândia-MG, 38408-100. solidonio@ufu.br

used directly in the generation of thermal and electrical energy (Sajid et al., 2022).

The syngas is produced in a thermochemical reactor. A fluidized bed reactor was chosen to be studied, as they have high operational flexibility, being able to work with a great heterogeneity of RDF, at different temperatures, gas residence times, reagents, catalysts and fluidizing agents (Arena et al., 2010). The ascendent flow during the gasification process carries small solid particles, which must be removed by cyclones to produce a clean gas.

In this research the cyclone is positioned inside the reactor. Therefore, the process of removing solid particles occurs at high temperatures (above 800oC), which contributes to prevent the formation of tar from condensable gases, increasing syngas lower heating value.

The cyclone separator is a device that uses the action of centrifugal forces to separate the dense phase of a multiphase flow (Karagoz, 2005), taking advantage of the inertial forces of the fluid and a cylindrical-conical geometry, it creates an ascending vortex that carries the less dense part of the mixture out of the device, removing the dense part that remains at the bottom of the cyclone.

Based on the fluid dynamic analysis of high temperature air flowing through a bed of sand inside the reactor, this work aims to analyze the efficiency of the axial cyclone in the removal of solid particles carried by syngas. However, in this work the thermochemical reactions inside the reactor will not be considered.

2. THEORY

This work is based on the previous study carried out by Ferrreira et al. (2021). In their work, these authors presented the mass and energy balances for a fluidized bed reactor on a semi-industrial scale (Fig. 1). The reactor operates in a steady state at 850 ºC transforming around 300 kg/h of RDF into around 700 kg/h of synthesis gas. Inside the reactor, the RDF is immersed in a fluidized bed of sand and, due to the high temperature, thermochemical reactions begin. The product is the transformation of solid waste into combustible gas containing CO, H2 and CxHy.

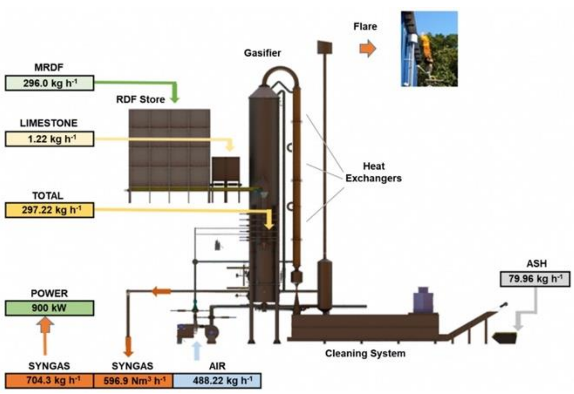

Figure 1. Mass balance applied to the thermochemical reactor.

Therefore, the present work aims to evaluate the particle filtration capacity of the cyclone installed inside the thermochemical reactor. A transient simulation of the fluidized bed on semi-industrial scale was done. The model considers the interaction between air and sand particles inside the reactor. The fluid dynamics inside the reactor and the efficiency of the axial cyclone in removing solid sand particles carried by the hot air were calculated.

2.1 Section titles and subtitles

Figure (2) depicts the geometry of the simulated thermochemical reactor.

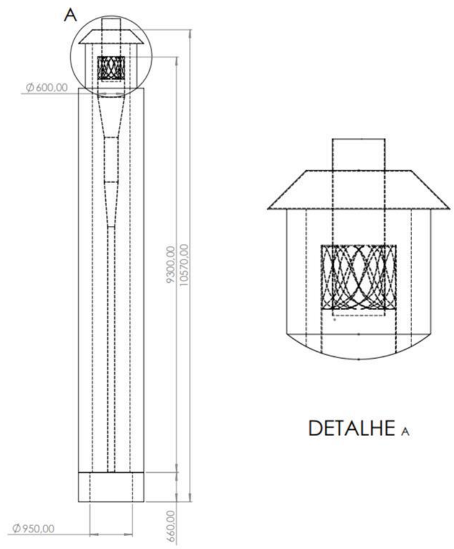

Figure 2. Thermochemical reactor geometry. Dimensions in mm.

In the Tab. (1) the dimensions of the equipment on a semi-industrial scale are presented.

Table 1. Dimensions of the simulated thermochemical reactor in mm.

Reactor Geometric Specifications	Size Value
Total height	10570
Internal diameter	950
Axial cyclone height	9300
Axial cyclone diameter	600
Height of cyclone blades	560
Fluidized bed height	660

One of the fundamental characteristics of the chosen thermochemical reactor is to have a high height so that, while the gas and its particles rise, the chemical reactions of catalytic breaking of the carbonic chains take place, which is extremely important for tar reduction and increase syngas heating value. The fluidized bed and the end of the cyclone are positioned at the lower part of the reactor (Fig. 3). Flowing through the bed the air lifts the particles that react with the hot atmosphere producing syngas.

The cyclone improves the quality of the gas produced in the reactor by separating the solid particles, at the same time it is a good option as it requires less constructive efforts and maintenance, in addition saving space as it is inside the reactor itself. In order to gain even more space, instead of using conventional (radial) cyclones, an axial one was chosen, as it presents an inlet area that will not require complex modifications in the reactor geometry. The upper part of the reactor in Fig. (4) demonstrates how the axial cyclone will be positioned.

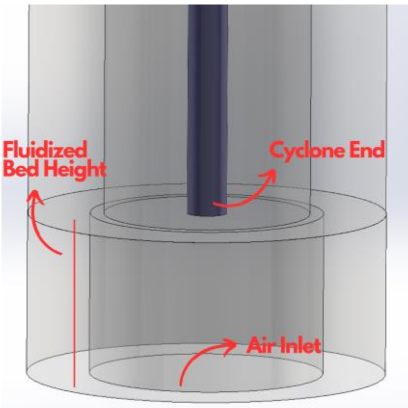

Figure 3. Lower part of the thermochemical reactor geometry.

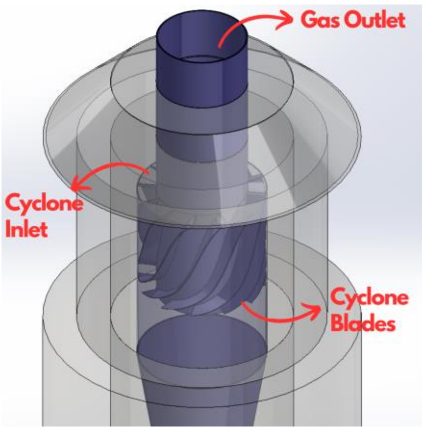

Figure 4. Upper part of the thermochemical reactor geometry.

There is a tradeoff in the cyclone design concerning the centrifugal acceleration and the pressure drop, the first one guarantee the separation of the mixture that flows into the cyclone and the second is an unwanted collateral effect. To solve this tradeoff twelve blades were designed to develop the vortex, these blades have a helical shape with increasing helix angle. This blade shape is responsible for the rotation of the gas stream that enters the cyclone, causing a centrifugal force that expels the particles (the densest part of the mixture) causing them to fall into its lower part, while the rest of the fluid escapes through the top.

2.2 The fluid dynamic model

To develop a computational model for the designed reactor, it was first necessary to extract the volume of the geometry, where the flow will be simulated, since the structural reactions are not relevant for this study. Then, using the interface ANSYS® Fluent (version 2023 R1), a finite element numerical model was developed, as well as the k-ω-SST turbulence model (Menter, 1994), which is the combination of the k- ω model (Wilcox, 1998) and the k-ε model (Launder e Spalding, 1974). According to Silveira Neto (2020), this formulation allows damping functions to be neglected for the solution of flows close to walls, which is convenient for the case of an internal flow.

In this way, some of the governing equations that support the model are determined, being the transport equation for the specific frequency of dissipation (ω) and the transport equation for the turbulent kinetic energy (k) (Eq. 1 and Eq. 2). In addition to the principle of conservation of mass, which ensures that the model is working properly (Eq. 3).

$$\frac{\partial \omega}{\partial t} + U_j \frac{\partial \omega}{\partial x_j} = \frac{\alpha \omega P_k}{k} - \beta \omega^2 + \\ + \frac{\partial}{\partial x_j}\left[\left(\upsilon + \sigma_\omega \upsilon_t\right)\frac{\partial \omega}{\partial x_j}\right] + 2\left(1 - F_1\right)\alpha_{\omega^2} \frac{1}{\omega}\frac{\partial k}{\partial x_i}\frac{\partial \omega}{\partial x_i} \quad (1)$$

$$\frac{\partial k}{\partial t} + U_j \frac{\partial k}{\partial x_j} = P_k - \beta k \omega + \frac{\partial}{\partial x_j}\left[\left(\upsilon + \sigma_k \upsilon_t\right)\frac{\partial k}{\partial x_j}\right] \quad (2)$$

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} = 0 \quad (3)$$

where, ρ is the fluid density, σ_k and σ_ω are turbulent Prandtl coefficients for k e ω, respectively, υ is the dynamic viscosity, υt is the turbulent viscosity, P_k is the turbulent kinetic energy production and the coefficients α, β, $\alpha\omega^2$, in addition to the mixing function F1 are empirical parameters of the model, u, v, w are velocities and x, y, z the cartesian axes. For the remaining constants, the ANSYS® k-ω-SST model configuration defaults were used.

As boundary conditions of the problem, an inlet velocity of 0.16 m/s was adopted, which represents an air mass flow rate of 500 kg/h, in addition to a null outlet pressure, allowing the calculations of the necessary pressure that the fan must be able to deliver for the specified flow rate. Furthermore, a mass of 0.279 kg of sand, with density equal to 1600 kg/m³, was added at 10000 points within a volume represented by 0.5 m of height, starting from the reactor bottom, uniformly filled with particles distributed by a Rosin-Rammler distribution pattern, where the diameters are ranging from 300 µm to 10 µm, with a mean diameter of 150 µm.

For this mass to be simulated, the Discrete Phase Model (DPM) was used. It presents a Eulerian-Lagrangian formulation, which works with the independence of the thermophysical properties between the two phases of the flow, where the Lagrangian frame of reference is used to track particles' motion, while the Eulerian formulation is used for tracking the continuous phase of the flow (Zahari et al., 2018).

The choice of this method promotes a simplified analysis of the expected results in the real process, since the real fluidized bed will present a much larger number of particles, however, it would require an excessive computational effort to enable its reproduction with DPM.

Understanding the principles of the simulation, it only remains to apply them in the reactor geometry, changing the temperature, density and velocity of the air entering the lower part of the reactor to 800°C, 0.3246 kg/m³ and 0.6036 m/s, respectively. Furthermore, the temperature of the entire system must be defined as constant.

In the simulation process, the numerical convergence of the 3D model was obtained considering the following parameters:

Table 2. Simulation Parameters.

Parameter	Value
Type of numerical mesh	Tetrahedral
Total number of cells	10,541,682
Time step, s	0.02
Total time simulated, s	40
Iterations per time step	5

3. THEORY

Based on Tab. (2), Fig. (5) shows the air velocity streamlines inside the reactor and axial cyclone, with a maximum velocity of 9.975 m/s, which is approximately 24 times the input velocity of the system.

Also, an inlet pressure of 54.035 Pa was calculated as well as the pressure contour as depicted in Fig. (6), furthermore the pressure in the axial cyclone head described an expected behavior, since it had negative pressure in the center of the cylinder, signaling that the flow should ascend in that region. To verify the validity of the data acquired a mass flow balance between the inlet and the outlet of the reactor was calculated, finding a negligible error percentage as shown in the Tab. (3).

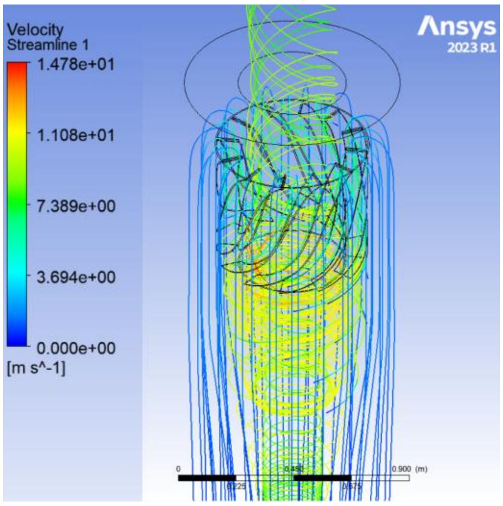

Figure 5. Streamlines according to the air velocity inside the reactor and axial cyclone.

Table 3. Mass Flow Balance.

Parameter	Value
Inlet	0.13880302
Outlet	-0.13880401
Net	-9.8805691e-07

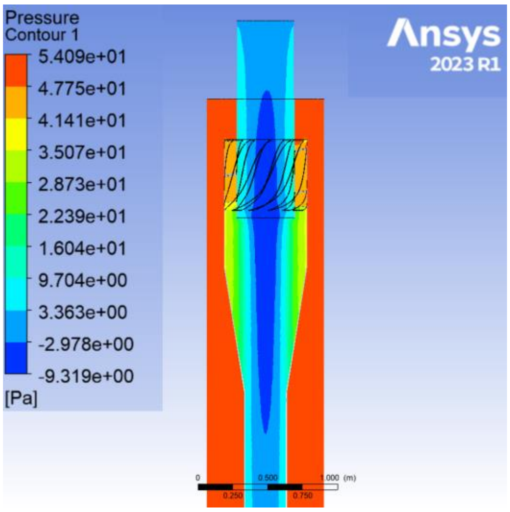

Figure 6. Pressure contour at the axial cyclone head.

In the tenth second, the smaller particles reach the cyclone inlet and their filtering process begins, as shown in Fig. (7). The largest particles being considered in the simulation, with diameters larger than 107 µm, remain at the base of the fluidized bed, and stop being graphically represented, to consume less computational resources.

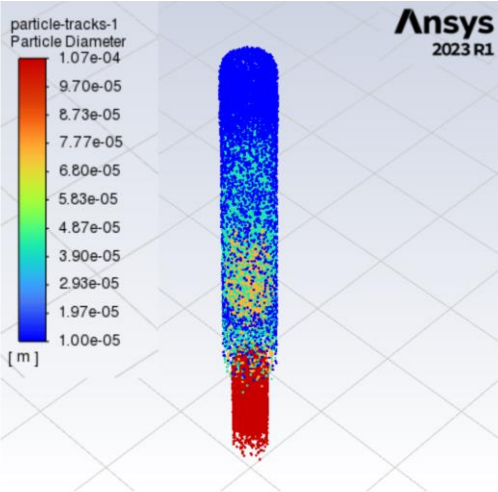

Figure 7. Behavior of the particles in the instant before entering the cyclone.

Figure (8) depicts the particle mass flow leaving the cyclone.

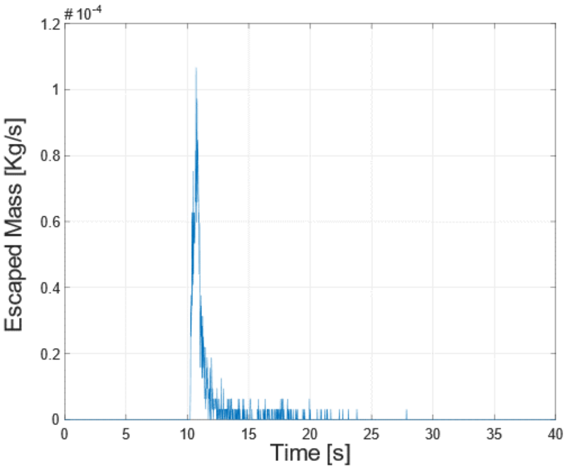

Figure 8. Mass of sand leaving the cyclone as a function of the physical time.

Applying an integral in Fig. (8), it is possible to verify that 72 mg of particles left with the air during 40 seconds of simulation. Heavier particles remain inside the reactor, returning to the base of the fluidized bed after passing through the cyclone. The total mass of sand that came out of the upper part of the cyclone represents 0.026% of the initial mass inside the reactor, proving the effectiveness of the axial cyclone in cleaning the air.

In Figure (9) it is possible to visualize, in the end of the simulation, the particles which remained inside the reactor. They are continuously filtered by the cyclone, descending in a rotational movement tangent to the cyclone wall.

The cyclone has an efficiency of 99.83 %, which proves that equipment was capable of filtering most of the particles and a clean syngas produced inside the reactor. Therefore, the main goal to gasify RDF in the reactor producing a clean gas with low pressure drop was obtained.

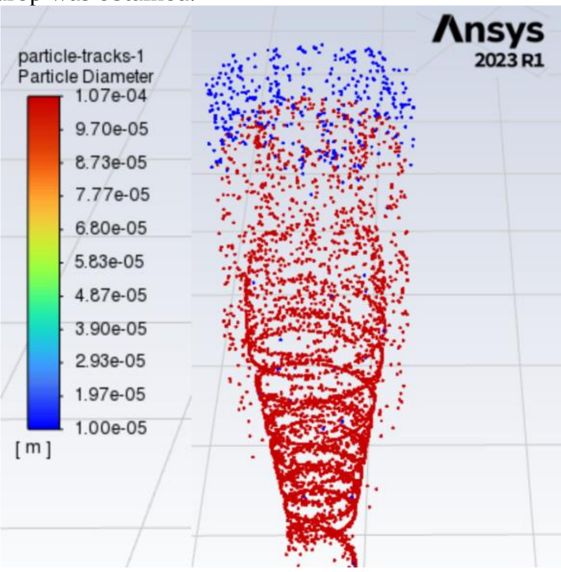

Figure 9. Particle behavior during filtering of larger diameter particles.

4. CONCLUSIONS

This work presents a study of the computational fluid dynamics of air and sand particles inside a semi-industrial scale fluidized bed reactor.

The mathematical and computational model demonstrated an excellent characterization of the proposed physical problem. Considering the mixture of air and sand inside the reactor, there was an efficiency of 99.83% in the cleaning process carried out by the axial cyclone, proving that this is a suitable equipment for the reactor.

For the simulation of the semi-industrial scale reactor, a Dell Precision T5820 workstation, Xeon W-2245, Ram 32GB, Quadro T600, SSD 512GB was required to carry out the simulations. The computational cost was 18 hours.

The next step consists of inserting the thermochemical reactions inside the reactor in order to simulate the gasification process of refuse derived fuel.

For future validation of the model, experiments will be carried out in a pilot plant at the company Carbogas Energia in Mauá - SP. In addition, a reactor on a scale equivalent to the one simulated in this work is under construction at the Federal University of Uberlândia. The experiments are scheduled for December 2025.

5. ACKNOWLEDGEMENTS

The authors acknowledge with gratitude the support of FINEP, FAPEMIG, CAPES, CNPq and the State Secretariat for Economic Development, Science, Technology and Higher Education of Minas Gerais (SEDE) for the financial support.

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