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Determination of fluid dynamic parameters through imports of CFD images validated in experiments for the MCNPX code.

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ABSTRACT

Nonintrusive gamma ray transmission measurements provided a significant contribution to flow structure models describing the FCC riser multiphase system. Circulating Fluidized Bed (CFB) in pilot cold unities are well-known facilities for parameters estimation. Two-phase is model approach to the fluid dynamic studies considering steady state in operational conditions. Flow characterization by semi empirical literature equations and CFD simulations are carried out in flow parameter estimation followed by CT gamma ray validation. In this work, the Monte Carlo simulation of gamma ray scan importing CFD experiments brings a wide range for the two-phase flow investigation. Computational methods are developed to interface geometry and dynamic functions describing circulating flow. Software implementation steps convert color scales into image grids corresponding to solid density. Therefore, the two-phase flow in CFD simulations was imported in MCNPX geometry. The Monte Carlo tomography simulation of three riser heights 0,65 m, 1,38 m and 3,42 m, yield volumetric fractions of 0,038, 0,013 and 0,004 for the solid radial distribution. The heights are of the three testing sections for monitoring pressure and gamma intensity. Results are compared to CT gamma ray tomography and to literature data.

Keywords: CT gamma, Importing CFD, Pilot cold unities, MCNPX, Validation.

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1. INTRODUCTION

Simulations with Computational Fluid Dynamics (CFD) have contributed significantly to the study of multiphase flow through numerical methods applied to fluid dynamics models. However, the complexity of the oil cracking process requires validation of the simulated data with experimental measurements performed in cold pilot plants that simulate the conditions of the industrial process: 1. The representativeness of the experimental data in function of the geometric and functional similarity of the pilot plant; 2. The scale-up process for the industry that may require the simulation of the innovation step obtained in combination with the simulation of the FCC kinetics.

The state of the art could be summarized, the different mathematical models used to describe the fluid dynamics in the literature, generate simulations that deviate from the behavior of industrial reactors and cold pilot units in the dense phase solids transport region. The solids recirculation problem is a challenge for the large number of FCC reactors operating in the world.

Each research group builds their cold physical model on a laboratory or pilot scale to study the process fluid dynamics and develops their research strategy. The approach to the multiphase flow through the two-phase air/FCC catalyst flow is the path established in the literature to measure fluid dynamics parameters.

Semi- empirical equations in the literature allow testing the values of the measured parameters and by comparing with similar works; the qualitative characterization of the biphasic flow can be characterized. Numerical simulations are used to solve the equations of the fluid dynamic models with parameters measured by gamma and X radiation transmission. A significantly contribution to define the structure of the flow and the precision in the velocities of the phases has been achieved by means of radioactive signals [1, 2]. The experimental limitations for pressure measurements are due to the disturbance in the flow caused by intrusive sensors. The source-detector arrangements for measuring radiation transmission have positioning limitations due to interference in the detection of scattering. Scanners require precision mechanics for design and installation and finally the cost of equipment and maintenance, might be taken into account.

The study of the biphasic system circulating in CFPU, proposed in this work aims to increase the capacity to validate the simulation through the integration of the CFD, MCNPX and Gama

Tomography methods. The realization of the proposal involves the import of CFD image into the geometry of the MCNPX and its more advanced step to import and simulate flow tomography that varies in time.

The validation of the integration of the methods requires the design of Data Flow in System [2] that in practice is the way of work in the CFPU based on the vast literature that interacts with CAD and MC [3, 4, 5].

2. MATERIALS AND METHODS

2.1. FCC type cold pilot unit

A Cold Flow Pilot Unit (CFPU) was designed and built to study the fluid dynamics of fluidized bed through the application of nuclear techniques and measured by pressure gradient (Figure 01). The project followed pilot plant requirements, scale up and objective: determine the hydrodynamics characteristics relevant to an FCC riser; combine these data with the results of other forms of investigation (CFD and MCNPX) and check the results of the model with data obtained in a commercial riser.

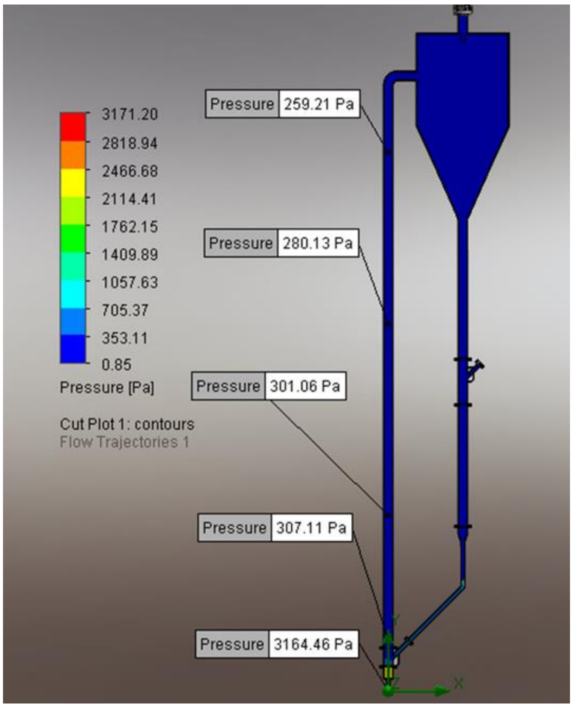

Figure 01: *Schematic View of the CFPU – Cold Flow Pilot Unit.*

The CFPU is composed of a vertical tube, called riser, with a 6,37 m height in polymethylmethacrylate (PMMA), a material better known as acrylic, the riser with 92 mm internal diameter and 100 mm of external diameter through which a biphasic mixture flows. Compressed air and cracking catalyst come into contact at the base of the reactor. The mixture rises through the riser in dilute solids transport regime and at the top of this segregates by the separation system, when passing to a chamber of diameter of the order of 15 times greater. Much of the catalyst returns to the lower part of the CFPU, while particles of smaller diameters are induced by the flow of compressed air to pass through a battery of 3 cyclones, still inside said separation chamber. Catalyst particles that are not retained by the cyclones are collected using a cartridge-type filter; similar to that used for air purification admitted by diesel engines. At the base of this filter there is a conduit in polyvinyl chloride (PVC) with the function of directing the finer particles, collected by another filter. The collected particles that leave the base of the separation chamber (flash) descend through a return column to a catalyst feedback system for the riser base. Figure 01 shows the operating scheme of the CFPU.

2.2. Parameter evaluation at the experimental pilot unit

Table 01: *Fundamental equations to investigate the two-phase flow*.

Equation/Parameter	Description
$\varepsilon_S = \frac{1}{(\rho_{p-}\rho_f)g}\frac{\Delta P}{\Delta Z}$ Industrial measurement	Volumetric fraction of solids, given by the difference on pressure, *ΔP*, involving a two-dimensional angle estimation with two separated sensors at a distance *ΔZ*, density variation of either particle or gas $(\rho_{p-}\rho_f)$ and g gravitational acceleration. Average value on *ΔZ*.
$\varepsilon_{sr} = \frac{1}{\rho_s\left(\frac{\mu}{\rho_s}\right)C}\, ln\left(\frac{I_E}{I_F}\right)$ Derivated equation	Radial distribution of the volumetric fraction of solids, given a mass attenuation coefficient, a correlation between the linear coefficient μ and the packing density of the solid ρ_s, the inner ropes length in the riser tube, C, and the gamma intensities of the empty and flow-induced riser I_F and I_E , respectively.
$C_S = \frac{\Delta P}{\Delta zg} = \rho_p\varepsilon_s$ [5]	Solids concentration in the riser, ρ_p is the density of the solid particle. Avarage value on *ΔZ*.
$u_s = \frac{\dot{m}}{\rho_p A(1-\varepsilon)}$ [1]	Kinetics in solids, ρ_p particle density, riser cross sectional area A, $(1-\varepsilon)$ volumetric fraction of the solids and solid injection through its mass $\dot{m}$ and time unit.
$v_s = u_g - u_s$ [1]	Slip velocity, given by gas and solid speed difference.
$\rho_{Nucleus}(x,y) = \begin{cases} 1, if\ \sqrt{x^2+y^2} < S \\ 0, if\ \sqrt{x^2+y^2} > S \end{cases}$	Nucleus-defined flow structure Coordinates: x and y, circle of radius S, whose center coincides with the center of tube at the origin

$\rho_{annul}(x,y) = \begin{cases} 1, if\ \sqrt{x^2+y^2} > S \\ m, if\ \sqrt{x^2+y^2} < S \end{cases}$ [6]	of the coordinate system.
	Flow structure set to annul m = (L - r) the length L of the inner riser string and r the radius of the circle S.

In Table 01, ε_S corresponds to (1- ε), where ε is the fraction of voids of a gas-solid bed, ρ density [kg/m³]. It is a measure of the axial distribution of the volumetric fraction of solids. It is an intrusive technique that causes disruption to the flow.

ε_{sr} is an equation based on Beer-Lambert, adapted for the tube-riser [7] and in which the diameter of the riser was replaced by C the length of the ropes in the case of the scanning tomography. It is non-intrusive measurement in the radial distribution of the volumetric fraction of solids.

The solids concentration, given in [kg/m³], is determined as a function of ΔP and is equated with the volumetric fraction of the solids.

u_s, also, can be calculated from v_s, considering the conditions proposed [1], we have:

$$v_s = \begin{Bmatrix} 0,\ if\ \ u_s\ =\ u_g \\ 0 < v_s\ \leq 5, if\ \ u_s\ \neq\ u_g \end{Bmatrix}. \quad (1)$$

Since the surface velocity of the gas given by $u_g = \frac{U}{\varepsilon}$, the slip velocity can be zero or is in the range of 1 to 5.

The core-annular structure of the flux [1] which was based on experimental measurements carried out with signals from radioactive sources; which for significate information's was obtained [8]. The formula for calculating the core-annular structure with data of the measurements with gamma transmission was defined [6].

The methodology developed with the equations in Table 01 led to the data presented in Table 02, and correlations that characterize the biphasic flow in riser whose results are published and represent the current knowledge of fluid dynamics at CFPU [9, 10, 11].

Table 02: *Physical properties and measured parameters at the cold pilot unit.*

Physical properties	Flow parameters
Pipe radius (r) → 0,092 m	Gas velocity → 1,76 m/s
Riser height (h) → 6,37 m	Solid velocity → 0,47 m/s
Particle mean size → 80 μm	*Slip* velocity → 1,29 m/s
Particle density → 1200 kg/m³	Solid volume fraction → 0,03
Bulk density → 850 kg/m³	Solids flux (W) → 28,77 $kgm^{-2}s^{-1}$
Solid → FCC catalyst	Backmixing → 7,03 $kgm^{-2}s^{-1}$

2.3. Gamma Ray Tomography by MCNPX Simulation

The simulation with MCNPX of gamma tomography in the study of nondestructive tests was optimized [12]. A further step was achieved by defining the limit of detection of the gamma tomography simulation method with the MCNPX for a static object [13]. The condition is implicit in Beer-Lambert equation [14] that equates intensity with linear attenuation coefficient for a gamma ray trajectory in a static system.

The CFD image import is a captured snapshot of an air-catalytic two-phase flow that changes over time. To continue the interaction with CFD, in addition to comparing radial flow distribution at the time, information is need to identify the experiment in which the snapshot was captured, and the comparison with experimental data is limited that image. The comparison with the steady-state flow and the system variation under study requires the import of the full experiment not only from the snapshot image. This is the computational problem of importing a dynamic object and then integrating the CFD and MCNPX simulations.

A working methodology was developed for the study focusing on the CFPU unit from a standard sampling with the operating conditions defined to evaluate all the experimental and simulated data. The methodology aims to calibrate and calculate the uncertainty of the entire integration methodology process.

As the flow is time dependent the motivation of the evolution of the industrial tomography was to improve time resolution. Therefore, from the first generation until the fourth and the instantaneous tomography, motivation focused on an instrumental solution. In the same direction the computational algorithms developed for reconstruction of the tomographic image prioritize the reduction of the number of input data by the reduction of the angles and trajectories in the scan. Dynamic tomography accesses the problem by searching for a mathematical model to decompose the mean value of the linear attenuation coefficient obtained at integration time t by the sequential values along of times $t_1, t_2, \ldots, t_n$. The most advanced initiatives of dynamic tomography come from algorithms for studying organs of the human body that work with contraction and expansion as heart and lung. However, an established methodology has not been reached and the dynamics is still object of study in the images to improve clinical tomography.

The investigation of the dynamic tomography led to the study of an adaptation of the Beer-Lambert equation:

$$I_f(t) = I_0 e^{-\bar{\mu}(x,t)dx(t)}. \quad (2)$$

With the final intensity and the mean attenuation coefficient $\bar{\mu}$ at time t, the values for the flux variations over t are calculated. The process of monitoring the variations occurred over time used simulated biphasic flow images in CFD in the study of dynamic tomographic reconstruction [15]. In the present work the estimation of the uncertainty must consider the steady state and the responses of the system the variation of a single variable in the process of static calibration [8], and in measurements of the dynamic system.

2.4. Selection of CFD files

The CFD images were obtained from three heights and represent different conditions of two-phase flow inside the riser. Produced through numerical simulations of the gas-solid flow and extracted from commercial CFD software, Fluent 15.0. ANSYS. Fluent is an international benchmark in fluid dynamics simulation studies. The results are represented by data referring to the volumetric fraction of solids in radial sections.

The images were validated by means of experimental [16] and compared with the MCNPX output data. It was through specific software, developed in previous work [13]. Information related to the radial distribution of catalyst in sections of the riser were extracted from the files generated by numerical simulations in computational fluid dynamics. Then, these are coupled to the code for simulation of the gamma-ray tomography with americium-241 source, allowing the subsequent obtaining of fluidodynamic parameters.

The CFD files selected for coupling in the code are represented by cuts in 2D slices, each slice corresponding to the determined height of the CFPU riser, with parameters, such as gas flow and constant solids. In addition, the images have RGB colors (additive color system: 'Red, Green and Blue'), to indicate the amount of catalyst in the studied radial section.

According to the CFD scale, used by software such as ANSYS Fluent and similar, the dark blue, present in the images, indicates a minimum volumetric fraction of solids. The colors in shades of green and yellow indicate, in this order, a volumetric fraction of solids increasing until reaching the dark red tone, indicative of the region with the highest concentration of solids.

The files with the volumetric fraction of solids in three sections of the tube simulate the following experimental parameters in the tube-riser: solids flow of 0,0620 kg/s, gas flow of 0,00834 m³/s and output of the mixture of 0,0725 kg/s. In Figure 02, these images are seen with the catalyst distribution at different heights, with heights of 0,650m (a), 1,384m (b) and 3,424m (c) all relative to the riser base.

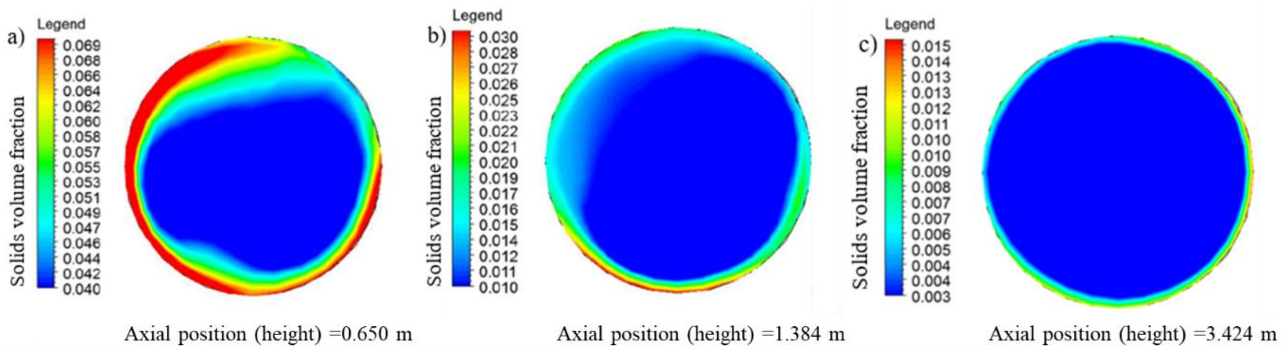

Figure 02: *Solid volumetric fraction distribution on the xy-plan at 0,65 m, 1,384 m and 3,42 m z-values.*

2.5. Importing image to MCNPX geometry

It consisted in the importation of gas-solid geometry through in-house software, whose main function is to extract data from CFD images and import into the MCNPX code, creating different catalyst and air distributions, variable with density [g/cm³], in radial sections of the tube-riser.

To import the CFD files into MCNPX using the insertion software, you need to perform a conversion of the standard RGB color tones present in these files o grayscale with a scale of 256 (0 to 255 tons). The import program uses the average of the different gray shades of the images to generate the catalyst distribution represented by small grids. Each grid contains density values [g/cm³] that vary according to the volumetric fraction of solids present in the CFD image.

In this way, a conversion software was developed in the Delphi environment, which has the function of turning the end tone darker to the white end in the grayscale scale and the darker blue to the black end of the same scale, of intermediate gray for the other colors. Figure 03 shows an example of the conversion done by the Software Converter.exe.

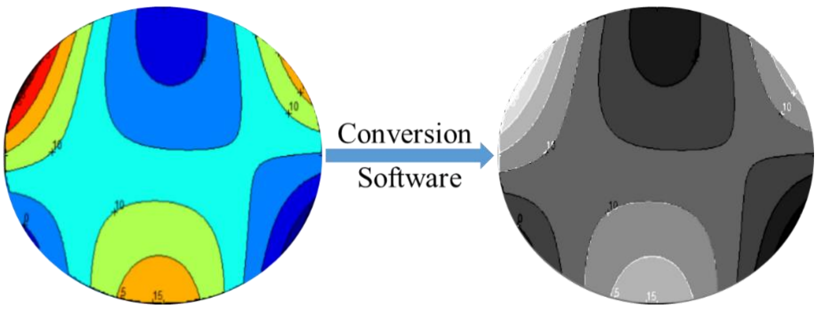

Figure 03: *CFD file conversion software for grayscale image.*

2.6. Importing software

Importing files representing radial riser sections without and in biphasic flow condition to MCNPX geometry. It was feasible due to the development of two import programs, one dedicated exclusively to inserting the air riser file and the other dedicated to inserting the air-riser into the code. The first was named *MCNP_Tomogama_Riser_Ar* and the second was *MCNP_Tomogama_Grid_CFD*.

Both were developed in Delphi language, being the first created in a previous work [13] and modified to perform the current simulations of airflow riser. And the latter developed in 2019 and later optimized to complete the current riser study with different solids distributions (Figure 04).

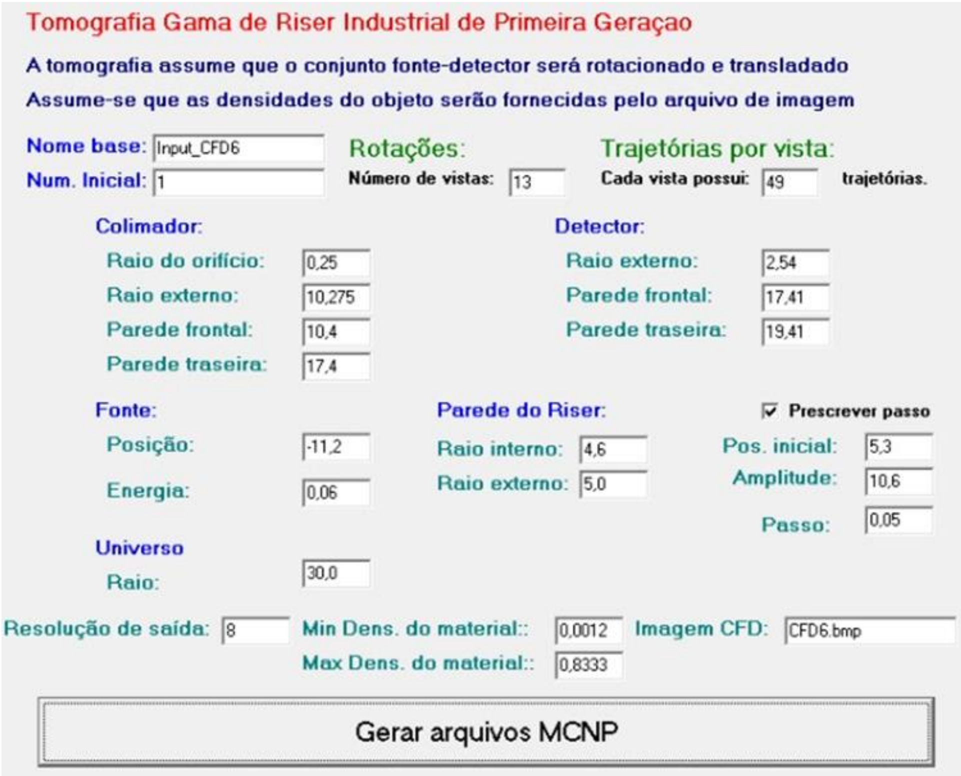

Figure 04: *Software interface MCNP_Tomogama_Grid_CFD.*

Its operation consists of importing the grayscale CFD image (converted) from the CFD image button, before inserting it, the user must rename the image to the name of his choice. Its operation consists of importing the grayscale CFD image (converted) from the CFD image button, before inserting it, the user must rename the image to the name of his choice.

Then it is necessary to choose the average density of the grids, with the minimum density corresponding to compressed air being 0,0012 g/cm³ and the maximum is usually the bulk density of the catalyst, which according to the experiment is 0,8332 g/cm³ [10].

However, depending on the imported image, this value may vary (calibration factor). Finally, the user can choose the output resolution from 1 to the ability of the code to run the files (12 outputs resolution). The increase in resolution is directly proportional to the increase in the amount of grids in the pipe section and inversely proportional to their physical dimensions. As a result, too high output resolution will result in a significant increase in simulation time. Thus, after several simulations, 8 (eight) was chosen as the ideal output resolution for this study.

After performing the tasks described in the previous paragraph, the user must click the Generate MCNP Files button. After this command, text files (INPs) will be generated with the grids, that is, the import process will be finished.

To view the riser section in MCNPX, native software vised.exe is used. In Figure 05, there is an example of importation ranging from the choice of the original image that can be validated or not by experiments (a), to conversion through software (b) and ending with the insertion and visualization of geometry in code (c).

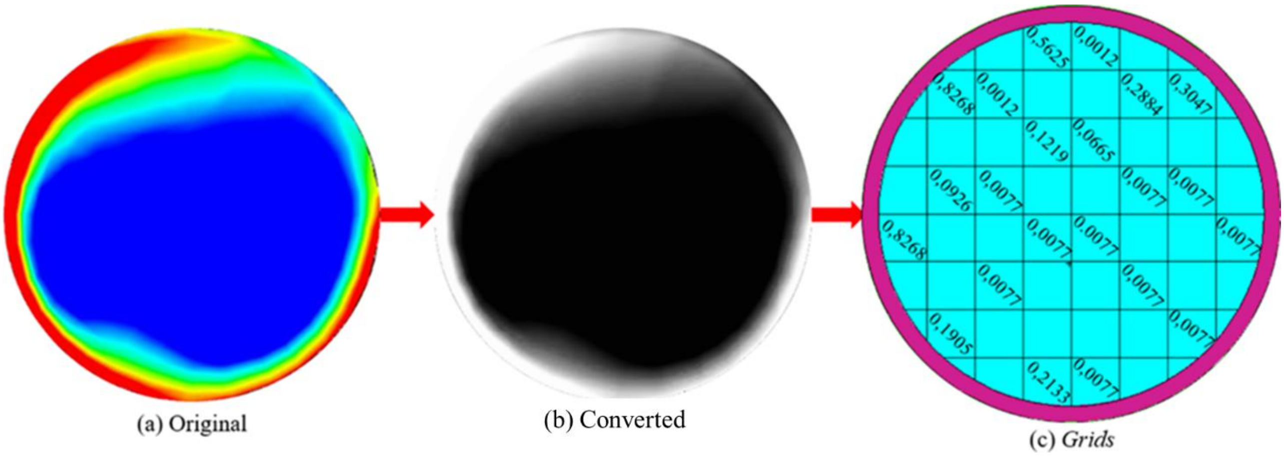

Figure 05: *Importing scheme by the software.*

To bring the real idea of how the interpretation of the import by the MCNPX code is made, in (c) some grids with their respective numerical density values were highlighted. That is, in Figure 05, it is observed that the geometry resulting from the import (c) is represented by large within the riser.

These grids have a geometric shape and varying density [g/cm³] of approximately 0,83 g/cm³, in parts where there is the largest volume fraction of solids (red in the original image or white in the converted image). Up to a minimum value of 0,0012 g/cm³, where there is a lower amount of catalyst (dark blue in the original image or black in the converted image).

In the case of the riser with compressed air inside, the *MCNP_Tomogama_Riser_Ar* software creates several files where the differentiation from one file to another is in the displacement of the source collimator and detector set along the x-axis of the tube (tomographic scan).

3. RESULTS AND DISCUSSION

The profile of the volume fraction of solids for three distinct sections was determined in MCNPX simulations. These images have the advantage of having their data extracted from Ansys Fluent and validated with experimental data from [16]. Through validation with experimental tomography technique, as demonstrated by [11].

Figures 06, 07 and 08 show radial profiles of volumetric fractions of solids obtained by simulations in Ansys Fluent [11]. Experimental data from the 1 Angle Scanning Gamma Computed Tomography (GCT - S1A) [16] and in MCNPX with simulations analogous to the experimental condition and 12 Angles Scanning Gamma Computed Tomography (GCT - S12A). Simulation data extracted from MCNPX tomography scanned over 12 angles, yielded a more detailed information from the radial distribution of the two phase flow in riser. Such a proceeding improves experimental single beam scanner at CFPU that is limited to one angle for each view.

Thus, 12-angle tomography allows the determination of a more detailed radial solids and gas profile, which opens the way for tomographic reconstruction of the section studied by specific algorithm [15]. In addition to allowing for a more in-depth quantitative assessment, it also allows a visual qualitative assessment of flow patterns.

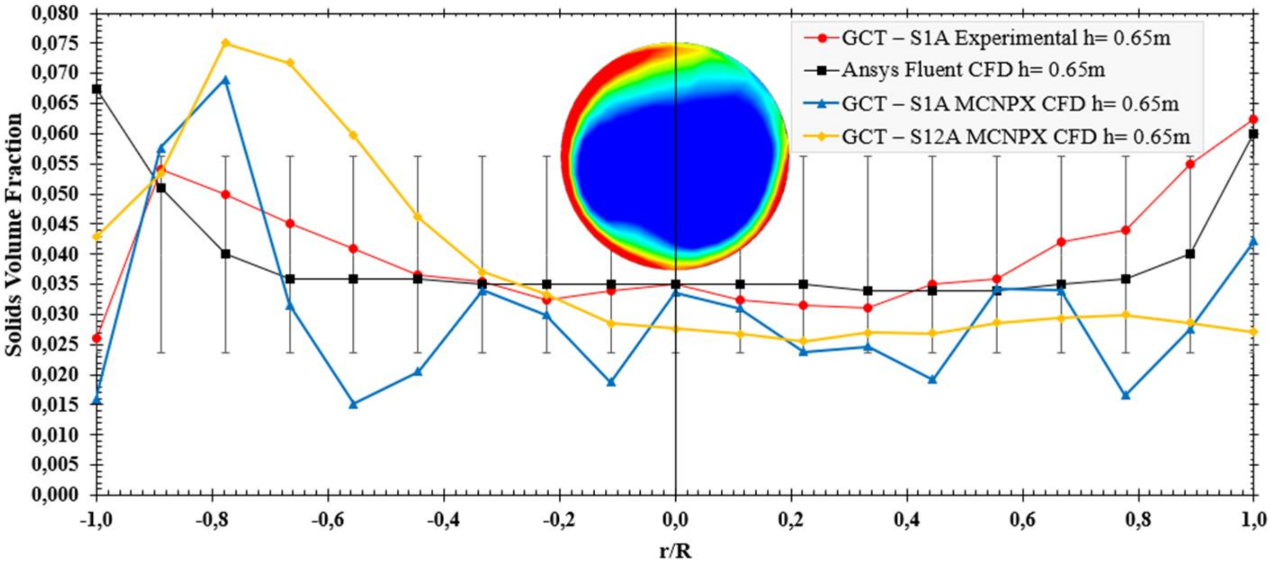

Figure 06: *Radial distribution of solids volumetric fraction versus normalized riser at the 0.650m height.*

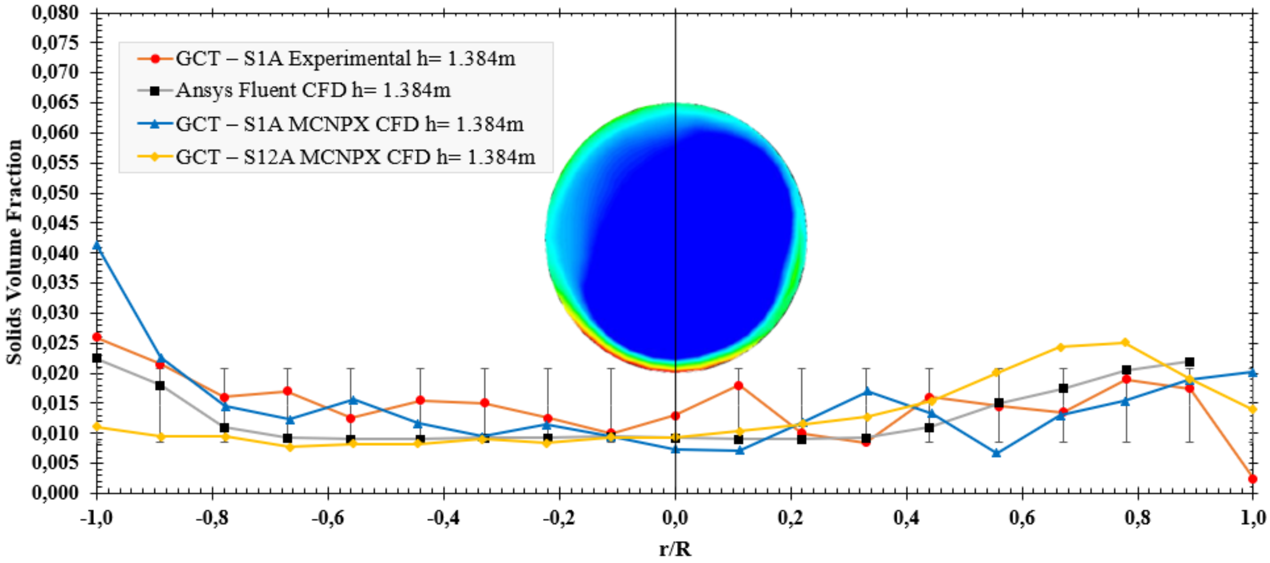

Figure 07: *Radial distribution of solids volumetric fraction versus normalized riser at the 1.384m height.*

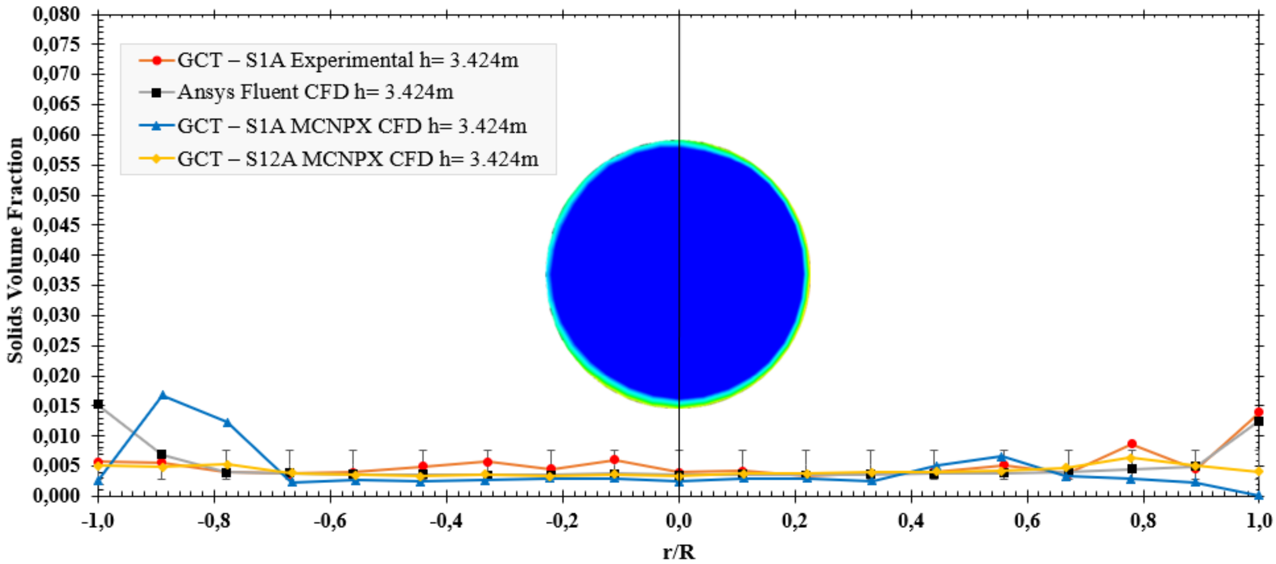

Figure 08: *Radial distribution of solids volumetric fraction versus normalized riser at the 3.424m height.*

In figures 06, 07 and 08 a comparison of the MCNPX tomography with Ansys Fluent data of the volumetric solid fraction radial distribution at three riser heights.

Higher concentration is observed near the riser wall and base, which decreases as the height of the measurements increases. Thus, through the mathematical modeling of the code output data, the radial profile of the volumetric fraction of solids was obtained, where three distinct regions with concentration gradients were identified.

The determined regions are in accordance with the flow pattern model proposed in the literature [7, 11, 17]. The initial riser portion (0,65m) is the densest region, characterized by its high turbulent intensities and asymmetric concentration caused by the region opposite to solids input. This explains the oscillation, especially in the region opposite solids output presented by the curve of volumetric fraction determined in the tomographic simulations.

In the fully developed flow region (1,384m), there is a less dense and approximately symmetrical region, which reflected in a radial solid fraction curve constant throughout most of the section. A small accumulation near the wall, which may be caused by a less intense downward flow, i.e., a low recirculation of solid. Near the top of the riser (3,424m) the solids concentration is much lower, with [7, 11]. It is currently being studied through the optimization of simulations in the Virtual Cold Pilot Unit and highly evaluated by research groups.

Therefore, in this region of the riser tube, the most stable radial solids profile curve with little variation over the radial section characteristic of the diluted flow regime is observed. From the radial profile of the volume fraction of solids, the curve of the solid axial profile along the riser is obtained as a function of its height.

The comparison between the axial profiles determined in the GCT simulation with 1-angle and 12-angle scanning is made (Figure 09). Where there is a differentiation in the volume fraction of solids present in the dense region and an almost zero difference in the diluted region.

Explanable due to the high sensitivity of 12-scan scanning angles for the region with the highest solids when compared to single-angle tomography. The axial profile of solids with the identification of three flow patterns is observed in literature data.

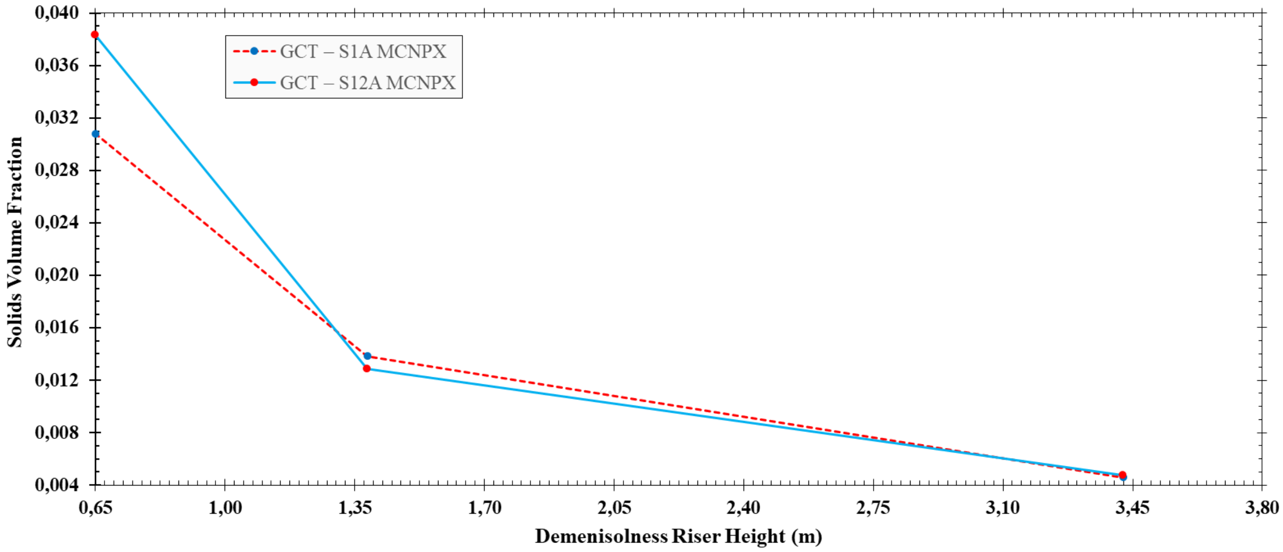

Figure 09: *Solid volumetric fraction against the three given riser height.*

4. CONCLUSIONS

The radial profiles of volumetric fraction of solids obtained with the simulations in the MCNPX code show good agreement with those obtained experimentally, via scanning by gamma transmission, and those obtained with the simulations in CFD. The software for importing CFD images is an important tool to correct errors in the interpretation of such images by the MCNPX code. In addition, the realization of simulations in MCNPX with scanning at 12 different angles expands both the experimental investigation, limited, since the experimental scan is made in a single trajectory, and the investigation through CFD simulations. As every industrial process values resource savings in all sectors in order to optimize production, the integration between the use of a simpler physical / experimental measurement system (first generation scanner - single scan trajectory) and a leaner one (installed in few measurement points), the aid via CFD simulations, which significantly contribute to the study of multiphase flows and provide images for a larger range of measurement points when compared to the experimental one, and the aid of simulations with the MCNPX code, proper when the process involves transporting radiation, corroborate this economy.

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