



# ROCKY

## Coupled Rocky-ANSYS Multiphase Flow Simulations Help Mitigate Coke Build-Up in a Petrochemical Pipeline



The petrochemical industry produces millions of tons of products per year that are heavily present in modern life, with wide applications in diverse sectors such as clothing, automotive, health, and others. In the olefins plants, equipment with great importance are the pyrolysis furnaces, which are responsible for thermally cracking naphtha, LPG, ethane, and recycle streams to produce the main products of the petrochemical industry including ethylene, propylene, hydrogen, gasoline, and pyrolysis residue.

One of the main problems of the pyrolysis furnaces is the gradual formation of carbon and hydrogen, known commonly as coke, in the coil walls of the furnaces. The equipment runlength is defined by the maximum temperature that the radiation coil walls reach during operation, which is caused by the coke being deposited onto the inner walls. Normally, the operation with high severity increases the production of the main product ethylene, but also increases the formation of coke and reduces the furnace runlength due to thermal and flow area restrictions. Therefore, the performance of the pyrolysis furnaces is critical for the economic performance of an olefins plant.

In order to eliminate the coke from the furnaces, it is necessary to interrupt the operation and submit the radiant coils to a process of decoking, which is the controlled burning of coke using a mixture of steam and air. Part of this coke does not burn and is mechanically dragged from the radiant coils accumulating upstream of the main Transferline block valve. When the furnace is put back into operation and aligned to the process (main Transferline), it flows as a plug of coke particles to the Primary Fractionator and Quench Oil Loop, resulting in filter obstruction (and sometimes damage), erosion problems, obstruction of Quench Oil Heat Exchangers, and even reduction in the plant capacity. Thus, the most efficient way to solve this problem is to avoid the deposition of coke, transporting it directly to the decoking pot during the decoke operation.

Braskem is the largest petrochemical company in the Americas and the world's leading biopolymer producer. This article explains how Braskem used ANSYS computational fluid dynamics (CFD) software to numerically replicate the geometry of the transfer line of the pyrolysis furnaces, evaluating the impact of the operational conditions and geometry on the velocity and pressure profiles and mainly on the prediction of the retained coke along the transfer line. The project aimed to evaluate the multiphase flow (gas and coke) in the transfer line of the pyrolysis furnaces during the decoking process to improve the efficiency process with minimal changes in existing geometries.

The mesh was generated in ANSYS Meshing with 650,000 tetrahedral and prismatic elements. Braskem ran ANSYS Fluent simulations assuming steady state and isothermal flow. The flow was treated as multiphase with a Euler-Lagrange one-way coupling approach and a SST turbulence model. Each simulation took 4 hours to run on a high-performance computing (HPC) platform with 12 cores.

The CFD analysis allowed Braskem engineers to identify coke deposition behavior under different operational and geometric conditions. As expected, higher gas flow rates resulted in lower retained particles percentage in the transfer line. However, for the particle size distribution considered, a small standard deviation was observed in the retained percentage for the larger particle diameters (3250 and 4000  $\mu\text{m}$ ), indicating that even with higher flow rates, the larger particles tended to remain in the domain. These results suggested that the system required geometric modifications for efficient particle removal from the transfer line, and that the operational conditions have a limited impact on the retained coke percentage. Figure 1 illustrates the velocity profiles for two different geometries.

## CHALLENGE

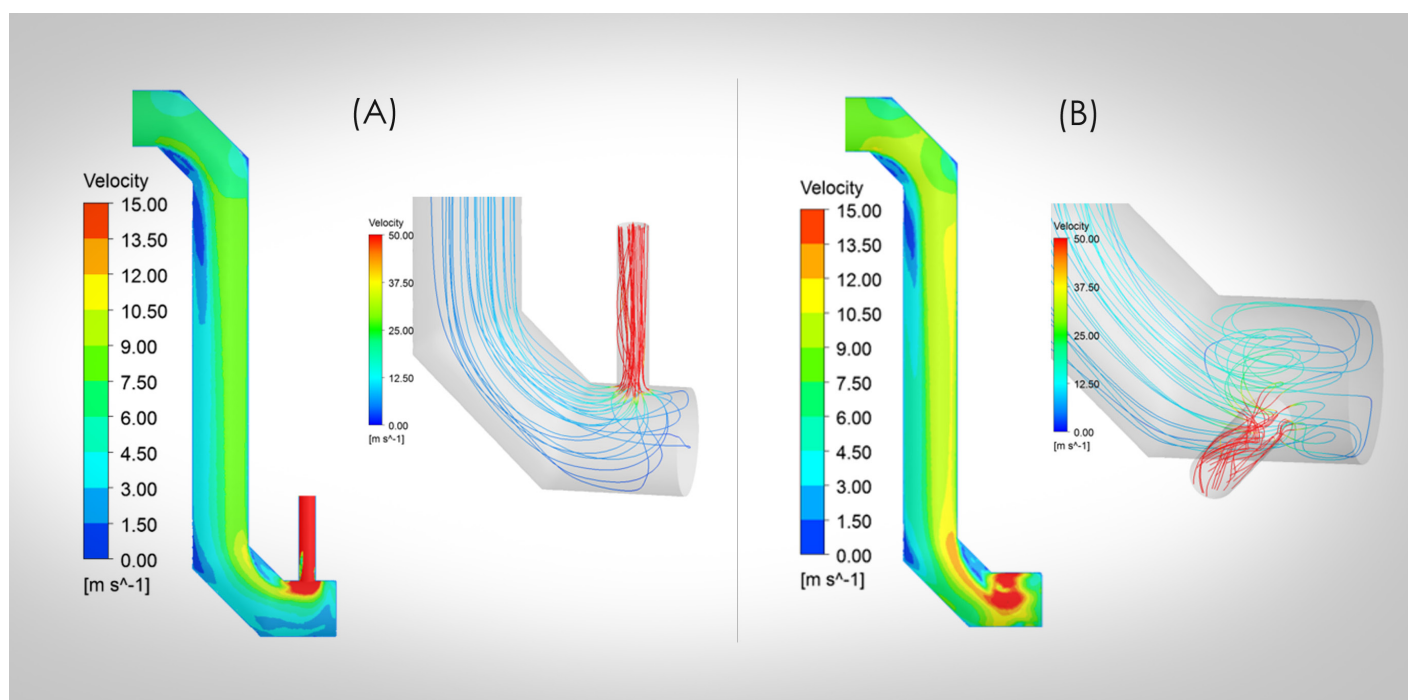
The gradual formation of carbon and hydrogen - known commonly as coke - in pyrolysis furnaces and pipelines was resulting in filter obstruction, erosion problems, obstruction of Quench Oil Heat Exchangers, and even reduction in the plant capacity.

## SOLUTION

Braskem used Rocky DEM and ANSYS coupling to numerically evaluate the behavior of multiphase flow (gas and coke) in the transfer line of the pyrolysis furnaces during the decoking process to improve the efficiency with minimal changes to existing geometries.

## BENEFITS

Rocky DEM and ANSYS simulations helped ensure the accurate prediction of multiphase flow behavior in order to avoid undesirable operational problems, save maintenance costs, and ensure safer operation of the equipment with greater efficiency.



◀ Figure 1 – Velocity profiles and streamlines for two different geometries in the transfer line: (a) vertical outlet pipe and (b) horizontal outlet pipe

The simulation revealed significant areas for improvement of the original design. Figure 2 shows the retained coke percentage for two different geometries by changing the outlet pipe layout. Due to some geometry restrictions, the changes in transfer lines were very subtle. The proposed modification consists of the rotation of the outlet pipe in

90° and it was observed that this simple modification reduced the coke mass deposition 90% in comparison with the vertical pipe case. The suggested geometry promotes greater velocity in the bottom of the pipe and consequently removes a larger amount of coke due to the reduction of recirculation and low velocity zones.

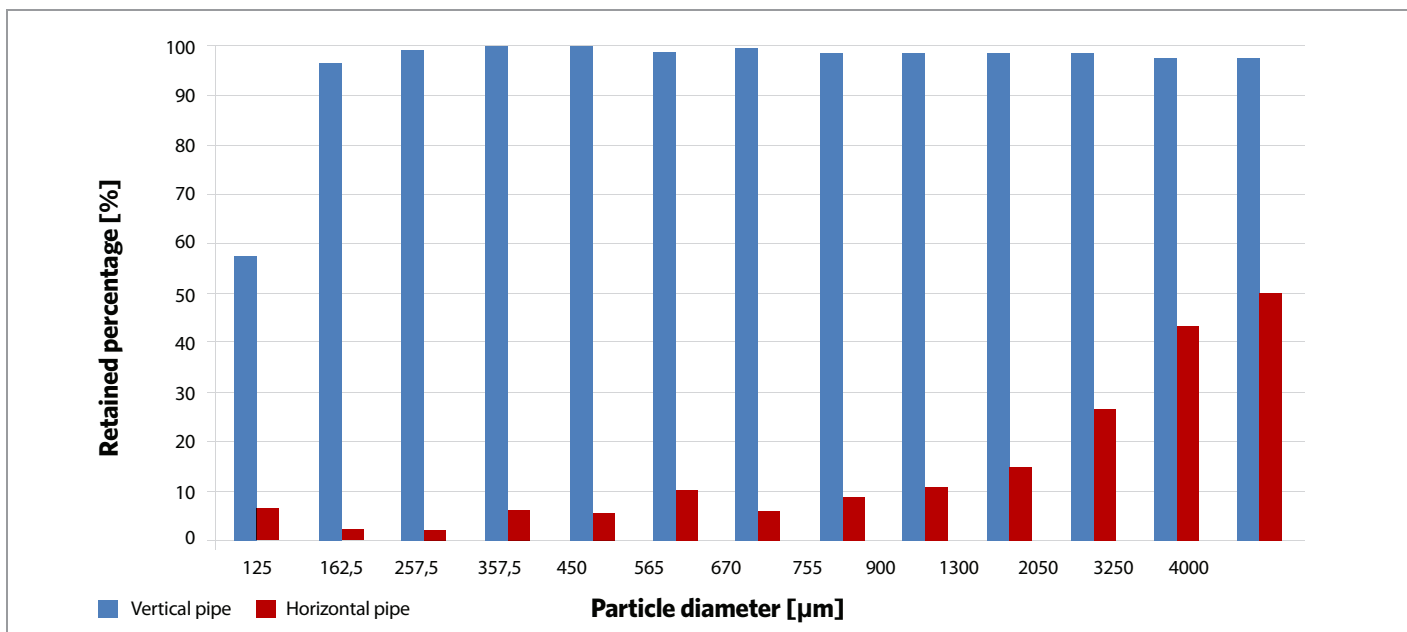


Figure 2 – Percentage of particle retained for two different transfer line geometries

In order to better predict particle behavior inside the line, a Fluent-Rocky one-way coupling simulation was performed, as it considers particle-to-particle and particle-to-wall interactions in a deterministic mode, despite the larger computational cost of this technology due to the greater number of particles (over a day depending on the number of particles tracked). This coupled simulation showed that the coke accumulates at the bottom of the transfer line, and at a certain position upstream of the main Transferline block valve, confirming the phenomenon observed in the actual industrial process. Figure 3 shows the results of the Fluent-Rocky coupling simulation, which illustrates the particle deposition locations.

The CFD and CFD-DEM models explained fairly well the impact of operating conditions and geometry changes on coke accumulation inside the transfer line. Furthermore, the use CFD-DEM coupling should be done for final quantitative verification, given a particle size distribution that better represents the physics involved.

This application demonstrates that fluid dynamic simulations can be used to predict multiphase flow behavior in order to avoid undesirable operational problems generated due to coke accumulation in the transfer line, saving maintenance costs and ensuring safer operation of the equipment with greater efficiency.

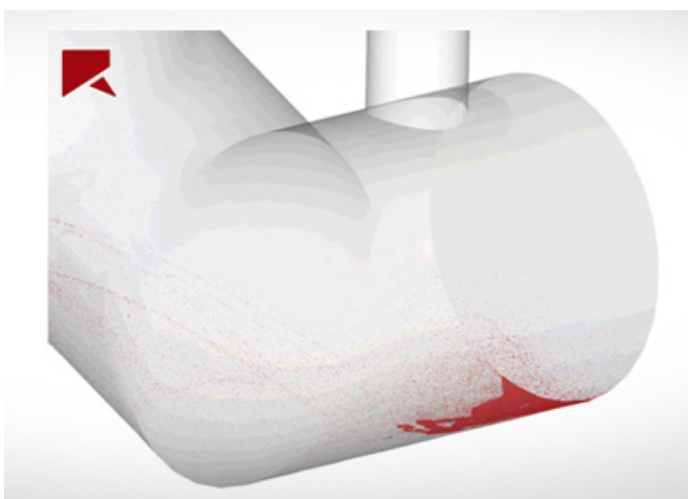


Figure 3 – Fluent-Rocky coupling results for the vertical outlet pipe geometry



Created in August 2002, today Braskem is the largest petrochemical company in the Americas and the world's leading biopolymer producer.

Braskem operates in the chemical and petrochemical industry and plays a significant role in other production chains that are essential to economic development.