

CASE STUDY

Ansys Rocky + Enerkem

Renewable Energy Sector "Wastes Not" with Rocky DEM Particle Simulation

"We have been using Ansys Rocky DEM for almost one year and have found it essential to our process: It has proved to be the only one with flexible fiber model coupled with CFD — flow solution and real representation of the particles, being able to analyze our equipment with the exact number of particles and format."

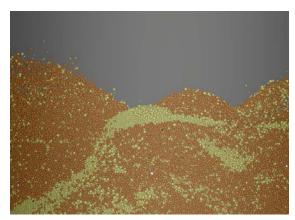
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CASE STUDY

Addressing altogether climate change and waste management challenges, Enerkem has developed an innovative process to produce biofuels and renewable chemicals from nonrecyclable waste. The company is offering an innovative, sustainable solution for waste management, energy diversification, and implementation of a circular economy, where waste becomes a resource for producing everyday products.

At the core of the technology lies a thermochemical process, called gasification, where an organic fraction of the waste is converted into syngas and separated from the inorganic part. This is realized continuously in a series of closed units involving solid handling, notably feeding system, fluidized bed reactor and inorganic extraction system. Produced syngas is then catalytically converted into biofuel.

As the frontline step of the process, gasification is required to produce a stable and good quality syngas. This should hold despite the heterogenous and variable nature of solid waste, which includes various organic fractions, woods, plastics, metals, and bits of rock. Adequate gasification is realized in a fluidized bed reactor, where a hot mass of sand is fluidized by mean of gaseous reagents. The heterogenous feedstock is continuously fed to the bed where it quickly mixes and



heats up, leading to its decomposition by pyrolysis followed by gasification reactions with the gaseous reagents. The mass of sand acts as a buffer, providing thermal inertia and holding the pool of feedstock into ongoing conversion.

Good control and design of the reactor requires understanding of its physics. The later involving multiple granular phases, multi-species gas phase, heat transfer, mass transfer, homogenous and heterogenous chemical reactions, mixing, segregation, large particle size distribution and a spectrum of fluidization regimes. It is a complex system, usually approached using labscale experiments, prototype testing, empirical calculations, and established best practices. Those approaches, although useful, have limitations and/or are costly.

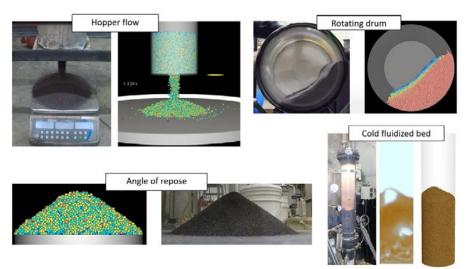


Figure 1: Calibration suite.

Driven by innovation, and continually seeking to push the boundaries, Enerkem engineers have been the forefront of adopting simulation technology. Various modeling approaches have been explored to simulate the fluidized bed gasifier, including two-fluid model (TFM), dense discrete phase model (DDPM) and multiphase particle-in-cell method (MP-PIC). They all proved, however, to be unsatisfactory for predicting friction regime behavior as well as segregation of multiple granular phases. Those physics are determining factors for specific functionalities or region inside the reactor, where a large spectrum of regime exists, from fixed bed up to turbulent fluidization. The limitations of those modeling approaches stem from their unresolved particle contact treatment.



Discrete element modeling (DEM), on the other hand, directly resolves the contact, and fills the above-mentioned fidelity gap. When properly coupled with CFD, DEM emerged as the only approach capable to predict the full physics spectrum at the required fidelity level. As Enerkem engineers were sorting through the various CFD-DEM offering, Rocky-DEM clearly stood out in terms of simulation speed. Its coupling with Ansys Fluent, to realize CFD-DEM, was also natural as the already established CFD tool at Enerkem. Ansys Rocky-DEM solver efficiency running on multi-GPUs was unmatched, surpassing codes running on large and expensive CPU clusters. It was now possible to run simulations with a larger number of particles and in less time. Also, Ansys Rocky-DEM fully supported coarse-graining model has been pivotal to promptly apply simulation at a large scale. Simulation of a reactor containing 10 tons fluidized bed and modeled with 25M coarsegrains are now practical and operational in the engineering workflow.

In general, Ansys Rocky-DEM was found to be a good balance between built-in capabilities and API hooks for customization. Its python scripting capability (pre-post API) is notably useful, as all routine simulations at Enerkem are now automated from pre- to post-processing. Large parametric calibration studies have also been easily automated using the pre-post API, as well as advanced post-processing, for computing mixing index as an example. On top of that, Rocky development team has been receptive and responsive to the specific application of Ansys Fluent coupling to fluidized bed reactor. Several new features have been developed and already released from this collaboration.

Eventually, it didn't take long before Enerkem engineers wanted to apply Ansys Rocky-DEM to other solid handling units, peripheral to the gasifier, like feeding system and solid inorganic extraction. Rocky usage quickly spread in other engineering projects, as the result of fast solver, ease to work with complex and moving geometries as well as powerful yet easy to use post-processing tool.

While Ansys Rocky is, as-is, "engineering production" capable, the recent release of the solver API opens a new world of possibility. Enerkem researchers now have their hands into the solver API, developing new models, like coarsegraining contact law and particle pyrolysis with mass loss, and are further raising simulation fidelity level.

/ CHALLENGE

As an emerging industry, converting trash into biofuels is laden with technical challenges. Analyzing granular and fluid flow in gasification reactor required physics simplifications and yet computationally expensive simulations that were not practical within a reasonable time frame. Enerkem traditionally used scaled-down CFD simulation models and bench testing to explore the domain, but more representative and faster tools and methods were required to support fast-paced innovation.

/ SOLUTION

Enerkem added Ansys Rocky-DEM particle software to its simulation toolkit, applying powerful capabilities to represent the gasification process more accurately, at full industrial scale and accounting for the right physics spectrum — in a realistic time frame. Leveraging new features like solver API allows the company to further tailor the software to the specific application of fluidized-bed gasifier.

/ BENEFITS

By quickly performing large CFD-DEM simulations with good fidelity, design options and operating scenarios can be virtually explored, leading to a better understanding of the process and to optimized reactor design. Applied in a troubleshooting context, the tool helps to diagnose problems and to guides to the right solution. Beyond gasification, Enerkem has started to apply Ansys Rocky-DEM to a wide range of solid handling equipment, peripheral to gasifier reactor, further supporting optimization of the gasification plant.

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