W H I T E   P A P E R - 1 0 6

The Role of Engineering Simulation in Clean Coal Technologies

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INTRODUCTION

In some circles in the United States, coal has become a dirty word. Among mainstream thermal power plants, coal has the highest emissions of carbon dioxide (the primary greenhouse gas) and, when the flue gas is untreated, coal combustion exhaust can also have higher levels of NO_X (nitrous oxides) and SO_X (sulfur oxides) emissions. Additionally, coal contains trace amounts of mercury, and it is believed that most of the mercury content in US lakes and rivers can be traced back to coal power plant emissions.

Despite the unprecedented development within the last 10 years of land-based gas turbines (running on natural gas), wind energy, solar energy, and even a renewed interest in nuclear power, on a pragmatic level, coal cannot be ignored in the United States. Figure 1 contains a chart showing the total coal reserves of the top eleven countries. The US has been referred to as “the Saudi Arabia of coal,” and from this data, it is clear that the name fits. If the US is to gain energy independence, coal must remain an energy source in the next 50 years.

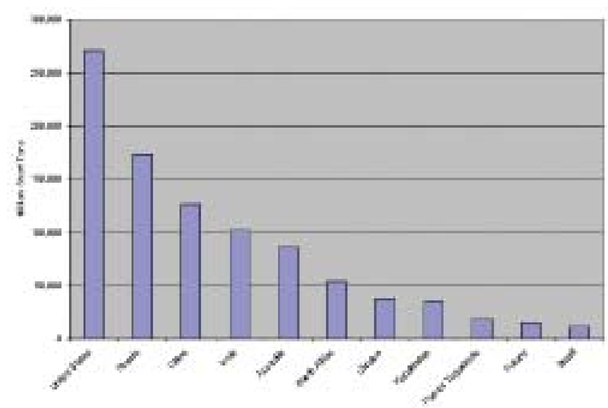


Figure 1: Coal reserves of the top eleven countries in the world
Source: DOE/EIA-0484, International Energy Outlook 2005

But can the environmental impacts be ignored? Figure 2 shows the annual quantity of carbon dioxide emissions (historical and forecast) for the top six countries. While the question as to whether or not carbon dioxide emissions cause global warming was uncertain ten years ago, the answer is now a resounding ‘yes,’ and the science has shifted to the matter of how much warming will occur. To stop the trend, carbon emissions need to decrease over time, but as the figure shows, all of the major emitters are continuing on an upward slope, with China on a particularly rapid incline.

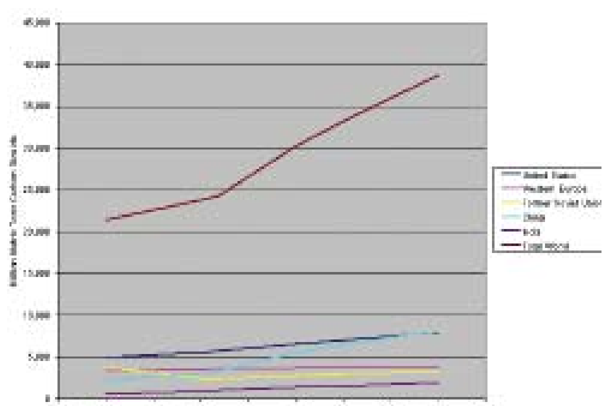


Figure 2: Carbon dioxide emissions from the leading emitting nations and the entire world
Source: DOE/EIA-0484, International Energy Outlook 2005

With the need to use coal-based energy, and the associated environmental dangers, what does the future hold? This white paper outlines the developing technology and shows the vital role being played by engineering simulation in ensuring maximum efficiency and environmental viability.

CLEAN COAL TECHNOLOGIES

There are three primary technologies competing to be the predominant next generation coal-fired power plant: Oxy-fuel combustion, Supercritical Pulverized Coal Combustion (SCPC), and Integrated Gasification Combined Cycle (IGCC).

Oxy-fuel combustion

All methods of oxy-fuel combustion separate the nitrogen in air from the oxygen before it reaches the furnace where it reacts with the coal fuel. While the purity of the oxygen stream may vary depending upon precisely which technology is used, the generation of nitrous oxides (NO_X) is significantly reduced, and the exhaust stream consists primarily of carbon dioxide and water, making separation of the carbon dioxide much easier than if significant nitrogen concentrations were present. The additional electricity cost for this methodology, however, is significant, possibly up to 40%. Nonetheless, it will remain a key technology, particularly for existing pulverized coal plants should carbon emissions be regulated in the near future.

SCPC

Supercritical pulverized coal combustion plants would use circulating fluidized bed combustion technology to raise the water temperature in high pressure heat exchanger tubes above the critical point. Large gains in efficiency and emissions reductions over existing pulverized coal boilers are attained through this technology, for a small increase in capital cost. The additional cost of electricity once the carbon capture capital is included in this system, however, is on the order of 65%.

IGCC

Gasification involves the highly controlled reaction of fuel with an oxidizing agent (air, oxygen, steam, or carbon dioxide) to form a carbon monoxide/hydrogen rich synthesis gas. This synthesis gas can then be used to drive a combined cycle gas turbine/steam turbine plant, or even a fuel cell. IGCC plants have a high capital cost (about 20% higher than today's pulverized coal plants), but the additional electricity cost for capture of carbon dioxide is just 25%. Additional features include the high plant efficiency and NOx removal capability of an SCPC plant, but with much higher rates of mercury and particulate removal.

THE FUTUREGEN PROGRAM

The FutureGen program, first announced by President Bush in 2003, is a $1 billion cost-shared project aimed at creating the world's first zero emissions combined electricity and hydrogen production plant using coal as a fuel source. The plant is envisioned to operate at 275 MW, sequestering one million metric tons of carbon dioxide per year, most likely in a combination of unmineable coal beds, depleted oil and gas reservoirs, deep saline aquifers, and for use in aging oil fields for enhanced recovery. The plant will operate a gasifier running on coal, water, and oxygen separated from air. The exhaust stream will first go through a gas cleaning process which separates sulfur and carbon dioxide, leaving a hydrogen rich stream to be used in a gas turbine, possibly coupled to a Solid Oxide Fuel Cell (SOFC), using a steam turbine in combined cycle, all generating electricity. Additional hydrogen can be generated for transportation. It is anticipated that the plant will achieve 99% sulfur removal, more than 90% mercury removal, emitting less than 0.05 lb/million BTU in NOx emissions and less than 0.005 lb/million BTU in particulates.

As a follow-up to FutureGen, the long awaited Energy Policy Act of 2005 contains significant funding and incentives for development of clean coal projects. This includes tax incentives on credit and cost sharing for gasification projects, as well as loan guarantees on projects that combine clean coal with other clean power generation technologies, such as wind and solar.

TECHNICAL CHALLENGES

While IGCC seems to be a very promising technology for the continued use of coal as an energy source while capping global warming, it does come at the price of increased capital. Emissions credits for carbon dioxide would likely make the investment worthwhile, and while the majority of the industry believes some form of carbon dioxide control is inevitable, opinions as to when this will occur vary widely.

On top of the cost hurdles, numerous technical challenges remain. Understanding ash behavior is a significant problem, particularly since IGCC plants include a series of large heat exchangers, where solids deposition, fouling or corrosion could cause expensive shutdowns. The formation of ash depends not only upon the coal type and particle size, but on complex processes that require knowledge of the complete temperature history of the particles during the gasification process. Deposition rates will depend upon the details of the exhaust flow through the heat exchangers.

Pressurized gasification complicates the coal injection process. This is usually dealt with through a lock hopper system or by using a water-based coal slurry feed. In either case, there is room for improvement and optimization. Another implication of pressurization is the need to depressurize by-product streams.

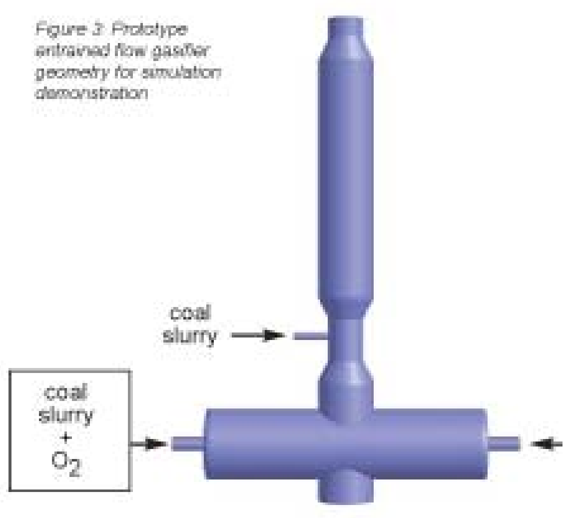
The two commercial scale IGCC systems now in operation (in Tampa and Wabash) do not remove emissions of pollutants and carbon dioxide to the near zero levels eventually anticipated. While it is well understood in principal how to accomplish this, the operational details need to be determined. The generation of a hydrogen stream in a FutureGen plant also requires further research and development. The hydrogen separation process will require the use of optimized membranes to ensure maximum energy efficiency.

HOW ENGINEERING SIMULATION CAN HELP

It is recognized that meeting the technical challenges faced by the FutureGen program requires state-of-the-art simulation capabilities. As such, the computational science group at the Department of Energy's National Energy Technology Lab (NETL) is working with collaborators to develop the Advanced Process Engineering Co-Simulator (APECS) , an integration framework that combines process simulation with high-fidelity three-dimensional equipment models employing computational fluid dynamics (CFD) technology. Coupling process simulation and CFD offers the capability to analyze overall system performance with respect to fluid flow, mass and heat transfer, chemical reactions, and related phenomena while maintaining accuracy in the representation of critical unit operations.

Perhaps the most critical unit in the IGCC system is the gasifier, and three-dimensional simulation can be used to investigate its performance under various operating conditions. The coal particle physics and chemistry that are unique to gasification have been built on top of the existing commercial combustion and fluid dynamics package, FLUENT. Demonstration of this technology has been performed by simulating the two-stage up-flow prototype entrained flow gasifier shown in Figure 3. It consists of a horizontal first stage and a vertical second stage. Coal slurry and oxygen are injected into the two side inlets of the first stage. This could actually be considered a coal combustor that provides hot gases through the connection to the second stage in which only coal slurry is injected. Most of the coal gasification process actually

Figure 3: Prototype entrained flow gasifier geometry for simulation demonstration



occurs in this second stage. Center plane contour plots of the resulting temperature field are shown in Figure 4, whereas key species concentrations are detailed in Figure 5. These images highlight the importance of three-dimensional modeling, showing clearly that properties cannot be considered uniform across the gasifier geometry.

Another type of gasification process takes place in the transport gasifier, in which air and steam enter from a bottom inlet, char recycle particles captured from the exhaust enter from a lower side inlet, and air and coal are fed from other side inlets. The coal particle concentrations are higher in this type of gasifier, with the gas "bubbling" up through the particle bed. While this requires more sophisticated modeling capabilities than the entrained flow gasifier, engineers are simulating these devices today. Some results of this unsteady process at one instant in time are shown in Figure 6.

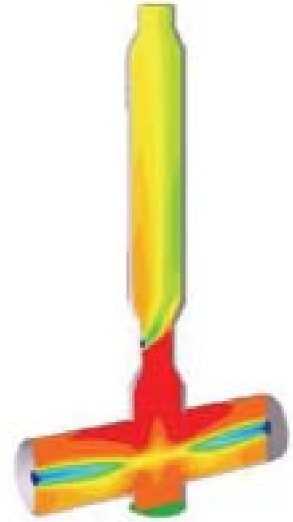


Figure 4: Contours of temperature computed inside the gasifier, with red representing the highest value and blue the lowest

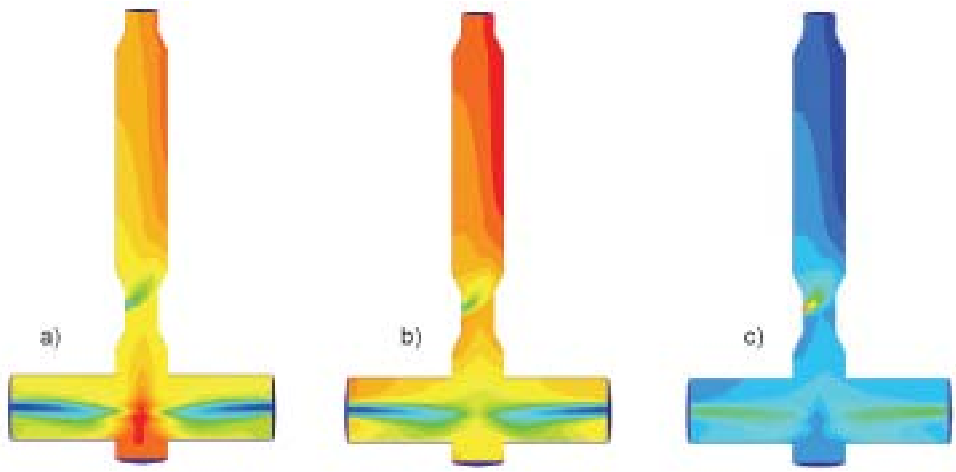


Figure 5: Contours of species mass fraction computed in the gasifier for a) CO, b) H_2, and c) H_2O

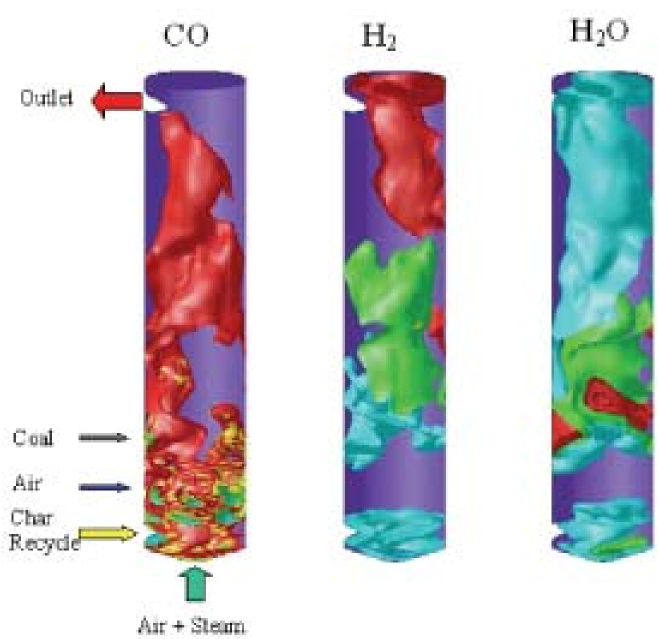


Figure 6: Isosurfaces of carbon monoxide, hydrogen, and water vapor from a simulation of a transport gasifier

SUMMARY

While today's coal plants contribute to the build-up of atmospheric carbon dioxide more than other traditional power plants, economics dictates that the US cannot control its energy future without coal. Existing technology will enable the use of coal while capturing not only the carbon dioxide, but also other harmful combustion byproducts, such as mercury, NO_X, SO_X, and particulates. The Department of Energy's FutureGen program is aimed at optimizing this technology, and a key aspect of this optimization process is engineering simulation. In particular, three-dimensional fluid dynamics simulation of critical unit operations, such as gasification, has been coupled to plant-scale process simulation. This capability will allow the rapid optimization of power plant design, ensuring maximum efficiency and environmental performance.

1 Zitney, S.E. and Guenther, C.J., "Gasification CFD Modeling for Advanced Power Plant Simulations," Proc. of the 22nd Annual International Pittsburgh Coal Conference, September 12-15, Pittsburgh, PA (2005).

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