GREEN ROUTES
Growing the bioeconomy
A GLOBAL manufacturer of gas turbines was facing the next round of international emissions standards that required a drastic reduction in pollutants including carbon monoxide and nitrogen oxides. The company turned to conventional computational fluid dynamics (CFD) but was limited by the very long run times needed to model detailed combustion chemistry. And when it tried to simplify and approximate the chemistry to get shorter run times, it no longer had the ability to accurately predict emissions. At that point, it could have resorted to physical testing, but real-world limitations in instrumentation, test stand availability and prototype hardware would have driven up the cost and resulted in significant delays to the schedule. Here, I discuss how reduced order modelling saved the day by solving the problem more quickly without compromising accuracy.

Turbine, boiler and furnace equipment designers are facing new challenges and new opportunities in today’s market that are driving them to seek more accurate and cost-effective design methods. Most manufacturers realise they need to account for alternative fuels, fuel flexibility and greater fuel and emissions efficiency in combustion-equipment designs in order to address new markets where traditional fuel sources are either scarce or unreliable. To date, adding fuel flexibility has involved considerable cost and extensive experimental testing. Reducing these costly and time-consuming experimental testing cycles needed to validate combustion performance is crucial to driving
development costs down. Minimising the risk of design mistakes identified after the sale reduces the cost of fixing them in the field.

Successful clean-combustion design is tied directly to the developer’s ability to integrate alternative fuels and fuel flexibility into the design; reduce emissions to stay ahead of environmental regulations; develop innovative technologies that increase efficiency; reduce the resources (cost and time) required to develop new designs; and improve the accuracy of emissions predictions that support performance guarantees.

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All of these factors drive combustion designers toward new design methods that allow them to achieve a substantial impact on fuel flexibility and efficiency, while reducing the resources and time required to design and test these new combustion systems. Using accurate simulation effectively is a key element that can help clean-combustion designers achieve these objectives.

The gas turbine industry’s ability to effectively use alternative fuels will have a large impact on future growth. To illustrate, consider a simple fuel such as natural gas. Natural gas composition is highly variable across geographic locations (see Table 1). In this era of tightening emissions regulations, tried-and-true simulation methodologies like CFD don’t provide enough accuracy to ensure a confdent, thorough understanding of the effects of composition variations of natural gas. To help manufacturers assess the effects of these variations, combustion simulation must provide seamless, integrated methods of linking familiar methodologies like CFD and the powerful, highly-accurate capabilities of detailed chemistry. The variations in gas composition elicit significantly different combustion performance in terms of stability and emissions. Figure 1 illustrates how nitrogen oxides vary with fuel for large gas-turbine engines used for power production. The investment is staggering when you consider that each data point in this ﬁgure represents a full combustion test that costs tens of thousands of dollars and weeks of development resources. Moving this test cycle into a highly accurate virtual test environment provides a faster, more cost-effective means of ensuring fuel ﬂexibility and lower emissions in new combustion systems.

**CURRENT COMBUSTION SIMULATION CAPABILITIES**

Combustion system designers have made great strides in recent years in developing low-emissions systems in the power and transportation markets, with minimal performance tradeoffs. In order to bring these new designs to market, combustion designers needed to move away from traditional build-and-test design processes. Experimental tests cost from tens to hundreds of thousands of dollars apiece and take months to complete – driving the need for new design methods. The development of low-NOx systems, such as dry low-NOx (DLN), lean premixed prevaporised (LPP) and rich burn-quick quench-lean burn (RQL), depended upon simulated combustion. Some of these new approaches often require the combustor or burner to operate closer to stability limits than in conventional combustion designs. So, developing fuel-flexible, advanced low-NOx designs still represents a significant challenge to the combustion designer.

Typically, combustion is modelled in CFD as the process of burning a hydrocarbon fuel in air to produce CO₂ and H₂O, represented by one, or a few, global reaction step(s). In fact, the process of combustion involves hundreds of short-lived species that participate in thousands of reactions while forming the products of combustion. These detailed chemical reactions are responsible for combustion stability and the formation of pollutants.

**TABLE 1: TYPICAL COMPOSITION OF NATURAL GAS**

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<table>
<thead>
<tr>
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<tbody>
<tr>
<td><strong>Methane</strong></td>
<td>CH₄</td>
<td>70−90%</td>
</tr>
<tr>
<td><strong>Ethane</strong></td>
<td>C₂H₆</td>
<td>0−20%</td>
</tr>
<tr>
<td><strong>Propane</strong></td>
<td>C₃H₈</td>
<td></td>
</tr>
<tr>
<td><strong>Butane</strong></td>
<td>C₄H₁₀</td>
<td></td>
</tr>
<tr>
<td><strong>Carbon dioxide</strong></td>
<td>CO₂</td>
<td>0−8%</td>
</tr>
<tr>
<td><strong>Oxygen</strong></td>
<td>O₂</td>
<td>0−0.2%</td>
</tr>
<tr>
<td><strong>Nitrogen</strong></td>
<td>N₂</td>
<td>0−5%</td>
</tr>
<tr>
<td><strong>Hydrogen sulphide</strong></td>
<td>H₂S</td>
<td>0−5%</td>
</tr>
<tr>
<td><strong>Rare gases</strong></td>
<td>A, He, Ne, Xe</td>
<td>Trace</td>
</tr>
</tbody>
</table>
Faster computers and better knowledge of fluid dynamics and combustion chemistry have allowed CFD to become integrated into the combustor design process and to provide valuable design assistance. However, CFD simulation run times are not fast enough to incorporate the detailed combustion chemistry of the fuel combustion. This is where reduced-order chemical reactor modelling approaches come into play. By simplifying the model, more detailed chemistry can be incorporated. Tools such as ANSYS’ Chemkin-Pro can quickly simulate the details of the combustion process using a fully accurate mechanism for the fuel oxidation with hundreds or thousands of species and reactions while simplifying the spatial geometry. The trick is to represent a complex 3D geometry and flow field as a series of 0D and 1D ‘reactors’ that allow you to apply accurate fuel chemistry mechanisms. This greatly simplifies the computations while preserving accuracy.

To accurately and cost-effectively incorporate detailed chemistry into combustion simulation, a method must bring together the best attributes of CFD and reactor modelling, as suggested in Table 2. This is done by carefully mapping regions in the combustor CFD solution, in which the cells have chemical similarity to discrete reactors and then accounting for all of the mass flow across region boundaries (see Figure 2) in a flow-connected reactor network.

**THE EQUIVALENT REACTOR NETWORK APPROACH**

Applying detailed fuel-combustion and emission formation chemistry in combustion simulation requires a simplification of the geometry. Equivalent reactors represent the combustor as a series of idealised reactors to allow use of detailed chemistry within an acceptable amount of computational time. Complex combustor geometry and flow can be converted effectively into an equivalent reactor network (ERN) that links the reactors together. Once the ERN is created through a careful processing of the combustor flow field, a fully detailed reaction mechanism can be used to provide the most accurate understanding of combustion behaviour and performance. For this approach to be successful, however, it is critical that the ERN is a true representation of the actual combustor flow field.

The successful use of ERNs to accurately predict emissions has been demonstrated in many studies for a wide variety of combustion systems. However, systematic ways of generating reliable networks have been elusive. One major drawback of applying this approach is that an expert in detailed chemistry typically takes several weeks to several months to create ERNs manually. When you consider the fact that there are now dozens of fuel types that equipment must accommodate in order to be successful, the need for a streamlined manner of using ERNs with accurate CFD for emissions predictions is obvious. The alternative of conducting experiments to evaluate the performance of so many fuels costs too much in money and time and, as previously mentioned, CFD cannot handle the detailed chemistry needed for accurate results.

ANSYS has developed the Energico simulation, unique in that it automatically creates ERNs from reacting-flow CFD solutions. It uses a series of filters or user-defined variables.

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**TABLE 2: COMPARISON BETWEEN CFD AND CHEMKIN-PRO REACTOR MODELING**

<table>
<thead>
<tr>
<th>COMPUTATIONAL FLUID DYNAMICS</th>
<th>CHEMKIN-PRO</th>
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</thead>
<tbody>
<tr>
<td>Detailed spatial geometry.</td>
<td>Full combustion chemistry details.</td>
</tr>
<tr>
<td>3D flow representation.</td>
<td>Accurate prediction of trace chemical species including pollutants and soot precursors.</td>
</tr>
<tr>
<td>Accurate prediction of mass flows.</td>
<td>Accurate ignition chemistry.</td>
</tr>
<tr>
<td>Accurate heat transfer.</td>
<td>Simplified spatial geometry and flow field.</td>
</tr>
<tr>
<td>Simplified combustion chemistry.</td>
<td></td>
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</tbody>
</table>
that are applied to the CFD to generate the ERN for accurate prediction of combustion performance, including exit emissions. An algorithm is used to divide the combustor flow field into zones that will form the basis of the ERN. Once this ERN is created, Chemkin-Pro is used to apply the detailed fuel mechanism and solve the ERN with accurate chemistry to simulate the emissions of trace species such as NOx, CO and unburned hydrocarbons. The ERN can also be employed in a parametric variation of operating conditions and fuel composition to determine how such variations would affect performance.

**ERN Algorithm Development**

An algorithm to create the ERN from the CFD solution applies a series of ‘filters’ to different CFD variables such as temperature, oxygen, and fuel. Once contiguous cells are grouped into zones based on these filters, Energico calculates the mass flow connecting each zone to each other zone, as well as the mass flow entering each zone from external gas inlets. Automating this approach creates significant advantages; rapid application of ERN algorithms allows the user to quickly evaluate the impact of algorithm variables and identify the optimum algorithm for the emissions target of interest. Furthermore, automatically applying the ERN algorithm ensures that the design is free from manual errors introduced that can affect the reactor-zone determination.

**Alternative Fuels Analysis**

The ability to predict emissions accurately from flow-field-derived ERNs has a significant impact on the ability to assess the impact of real and alternative fuels. Alternative fuels can be modelled using the same approach that was described above. A CFD solution can be developed with global or dramatically-reduced reaction mechanisms that approximate the thermodynamics of the alternative fuel of interest.

From this solution, an ERN can be derived where a fully-detailed reaction mechanism for the fuel, or a reasonable fuel surrogate, can be applied in a computationally efficient manner.

**Assessing Lean Blow Off**

Low NOx-emission combustors utilise reduced peak-flame temperatures within the combustor to limit the formation of thermal NOx, through staging strategies such as lean, premixed combustion. As combustion temperatures are decreased in low-NOx applications, several other undesirable combustion phenomena become more prevalent and must be addressed. The low-NOx limit is often bounded by the onset of combustion instability in the form of lean blow off (LBO). LBO occurs when the thermal energy generated by the burning fuel/air mixture is no longer sufficient to heat the incoming fuel to the ignition point.

**Accurate Damköhler Numbers Are Important To Characterise Whether Diffusion Rates Or Reaction Rates Are More Important For Defining The Chemistry Throughout The Reaction Chamber**

Energico uses an innovative method to address the issue of defining Damköhler numbers (which relate the reaction rate to the transport phenomena rate occurring in a system) for a combustor, that takes advantage of the local flow and thermochemical properties extracted from a CFD solution and the kinetics available in the detailed chemistry mechanism. Accurate Damköhler numbers are important to characterise whether diffusion rates or reaction rates are more important for defining the chemistry throughout the reaction chamber. Rather than trying to define a pair of ‘global’ chemical and flow residence times for a whole combustor, the software’s LBO analysis tool defines both chemical and residence times locally to account for the spatial variation of mean flow, turbulence, and...
The LBO analysis verifies the integrity of the flame locally and provides an indication of the overall soundness of the flame zone visually, expressed as contours of the local Damköhler number. The Damköhler number distribution exposes the location and the size of the stable flame core in the combustor. By examining the structure and topology of the flame core and the integrity of the flame, the likeliness of blow-off can be determined. The adequacy of the CFD mesh for flame predictions in that area can also be assessed. An example of LBO results for a wall-jet can combustor is shown in Figure 4, where regions with a Damköhler number of greater than unity (blue regions) indicate regions where the flame is unstable.

**SOME SAMPLE RESULTS**

Figure 5 shows a comparison of Energico emissions results with experimental measurements for a single fuel injector from a low-NOx, industrial, gas-turbine engine. The injector is a well understood design and has significant experimental data that have been validated by the manufacturer. The experimental data are from single-nozzle combustion tests in an isolated rig and include the effects of fuel/air variations on exit-NOx emissions. As can be seen in the figure, the tool predicted the NOx emissions at the baseline point. Moreover, parametric variation of the ERN inputs to increase fuel/air ratio (ie increase combustor exit temperature) yielded NOx predictions that are in excellent agreement with the experimental results. The simulation was conducted in a couple of hours and its results can be used to replace a physical experiment that costs upwards of US$100,000 to perform.

**HOW REDUCED-ORDER MODELLING SOLVED THE GAS TURBINE EMISSIONS CHALLENGE**

Remember the gas turbine manufacturer? It decided to adopt a reduced-order modelling solution. Now it can run simulations very quickly, with the full, uncompromised chemistry, and it can now obtain accurate predictions of carbon monoxide and nitrogen oxides, allowing it to reduce experimental testing.

**REFERENCES**

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