2nd Oxyfuel Combustion Conference

Evaluation of the GERG-2008 Equation of State for the Simulation of Oxyfuel Systems

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1. Introduction

The design of power plant systems requires a considerable amount of modelling and simulation. Thermodynamic property models or equations of state that are used to describe the volumetric, energetic and transport behaviour of fluids involved such as flue gases, steam and cooling water are always applied. Most of the former projects in the power plant industry could be realized with only a few relatively simple equations of state because the fluids involved displayed almost ideal behaviour (except water for which quite complex equations were developed decades ago).

The situation is completely different for Oxyfuel power plants. The additional processes and units that are needed to operate an Oxyfuel power plant (air separation units, flue gas cleaning systems, purification units, compressors and others) are always dealing with complex fluid mixtures with strong real-gas behaviour and very different parameters (e.g. supercritical CO_2). Calculation of these processes using the simple "ideal" equations will produce relatively large errors, if it is even possible at all.

Therefore more sophisticated equations of state that are capable of representing the complex behaviour of the fluids need to be used. Ideally, a single equation of state would be used for all relevant processes. This would have the advantage of consistent results and numbers, especially at the interfaces of the different parts of the power plant. Additionally, this could lead to a smaller number of software packages that are used in the overall concept and design of new power plant projects.

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2. GERG-2008 Formulation

One of the mentioned equations of state is the GERG-2008 [1] formulation that was originally developed to calculate the thermodynamic properties of natural gas mixtures. The advantage of this formulation is the (theoretical) ability to provide consistent thermodynamic property data for the most relevant processes in an Oxyfuel power plant. Whether this is true for all conceivable cases and all relevant ranges of pressures, temperatures and mixtures will be discussed in the presentation.
The GERG-2008 formulation is an equation of state to calculate thermodynamic properties of mixtures with natural gas components. These components include:

- Methane (CH_4), Nitrogen (N_2), Carbon Dioxide (CO_2),
- Ethane (C_2H_6), Propane (C_3H_8), Butane (C_4H_{10}), Isobutane (C_4H_{10}), Pentane (C_5H_{12}), Isopentane (C_5H_{12}), Hexan (C_6H_{14}), Heptane (C_7H_{16}), Octane (C_8H_{18}), Nonane (C_9H_{20}), Decane ($C_{10}H_{22}$),
- Hydrogen (H_2), Hydrogen Sulphide (H_2S), Carbon Monoxide (CO), Water (H_2O), Oxygen (O_2), Argon (Ar) and Helium (He).

The extended range of validity is -153.15 °C to 426.85 °C at pressures below 700 bar if a higher uncertainty of results is acceptable. Extrapolation behaviour is reported to be good and some examples will be presented later. The equation is applicable to gaseous, liquid, supercritical and vapor-liquid equilibrium states for any mixture with the above-mentioned components, leading to the ability to use it in the simulation of very different processes.
The GERG-2008 formulation is an extension of the former GERG-2004 [2] equation (which is an international reference equation for natural gases) and is currently under preparation for adoption as an international standard (ISO 20765-2 und ISO 20765-3).

3. Capabilities for Process Simulations Using GERG-2008

The GERG-2008 equation could theoretically be used to derive thermodynamic properties for modelling and simulation of many different processes. In the special case of Oxyfuel power plants these applications include:

- cryogenic air separation units
- flue gas systems (boiler, flue gas treatment units)
- water/steam cycles
- CO_2 processing units

Usage is restricted by the constituents of the flue gas that have to be considered in the calculations. For example sulphur dioxide, a typical flue gas component, is not covered by the equations. Another restriction is the absence of equations describing the transport properties.
A number of other advantages and disadvantages relating to Oxyfuel systems in particular will be presented at the conference.

4. Comparison to Measurement Data and Other Equations of State

A large quantity of measurement data was used for fitting the parameters and coefficients of the GERG-2008 equation. Any lack of measurement data will therefore directly influence the uncertainty of the calculated values, which is especially true for mixtures. Because the equation uses binary interaction equations of different kinds some mixtures are represented more accurately than others, depending on the amount of reliable measurement data for the binary mixture. Especially for mixtures consisting mainly of minor natural gas components like carbon dioxide, oxygen, water and others, there were fewer measurement data and less complex equations were used for fitting.
Therefore it should be tested whether a given mixture is represented with acceptable uncertainty by the GERG-2008 equation. For the Oxyfuel application five different fluids or mixtures of fluids will be examined:

- air (standard air) under conditions of air separation units
- flue gas (Oxyfuel conditions)
- liquefied flue gas (as can be found in purification units)
- CO_2-rich, purified flue gas (pipeline conditions)

- water and steam (steam cycle conditions)

For each of these mixtures a typical composition will be examined and properties calculated using results from the GERG-2008 equation will be compared with measurement data and results from other general equations of state, e.g. the Peng-Robinson -Equation [3], the BWRS- Equation [4], the SRK equation [5], the PSRK equation [6] or special equations, e.g. for water [7] or air [8].

5. Software Packages Using the GERG-2008 Formulation

To date, only one process calculation software program (Aspen-HYSYS [9]) using the GERG-2008 equation as a possible source of thermodynamic properties is known to the authors. The authors of the GERG-2008 provide the equation of state as an add-in for Microsoft EXCEL® [10] and in the form of a DLL and therefore it is quite easy to implement this equation into other software packages.
Another widely-used software program providing access to the equation is REFPROP® [11], the Standard Reference Database 23 from NIST in Boulder. After adoption as an international standard it is expected that the number of programs supporting GERG-2008 will rapidly increase.

6. Conclusion

The GERG-2008 equation of state and its application in software programs used for modelling and simulation of different parts in Oxyfuel power plant systems will be presented in the speech.
This includes examining the performance of the equation in relation to several measurement data, other common equations of state and general practicability in typical engineering works, planning and design processes. Typical advantages of the equation will be shown and cases in which other equations should be used will be discussed.

7. References

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