EXTENDED MATERIAL PROPERTIES IN APROS FOR DEPENDABLE EVALUATION OF NEW COMBUSTION POWER PLANT CONCEPTS

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Abstract

Sustainable power production requirements call for extended ranges and more detailed accuracy in calculation of material properties in dynamic simulation of new designs of combustion power plants. Better thermal efficiency may be gained from increasing the steam temperatures to the over critical region. More detailed calculation in condensers requires also non-condensable gases to be considered in the steam and water circuits. Carbon capture and storage (CCS) concepts require that the flue gas circuits can include liquid carbon dioxide calculation. Oxy fuel concepts require separation of oxygen and extension of the material properties of air with liquid nitrogen and oxygen. Versatile use of dynamic simulation in design evaluation of such novel power production concepts require fast and accurate calculation of the material properties. The APROS thermal hydraulic solvers provide information on pressure, specific enthalpy, and mass fractions of mixture in each control volume as input for the material property calculations. The material properties calculated include the temperatures and void fractions of each control volume as well as the properties needed for each phase such as the mass fractions, densities, viscosities, specific heat coefficients and specific enthalpies. Extended range calculations of the material properties, as well as example applications, are presented.

Keywords: modelling, dynamic simulation, power plant, material properties, APROS.

Presenting Author's biography

Dr. Kaj Juslin studied Electrical Power Engineering at Helsinki University of Technology (HUT) for his master's degree. His postgraduate interests concerned Control Theory and Electrical Engineering Theory. He has held many different positions at VTT Technical Research Centre of Finland, already since 1970. His present titles are Customer Manager and Chief Scientist. He has been responsible for the co-ordination of several research initiatives related to dynamic simulation of industrial processes. He is the main architect of the APROS software, now in extensive use world wide. He has promoted international cooperation acting as president of SIMS and EUROSIM.

1 Introduction

Simulation has traditionally provided an economically feasible test bench, when some production technology is pushed to new area, unknown for industrial experiences. Naturally this also sets a challenge for simulation providers, because tools tend to be designed for the tasks and needs at hand. It is known that material properties play key role in producing reliability for the simulation results. Accordingly, novel technology concepts within combustion power industry inspired the developers of the APROS modelling and dynamic simulation environment [1] to extend the adapted material property calculation [2] to meet the new requirements.

The efficiency of a power plant can be considerably increased if the process can be operated in elevated temperature and pressure. Thus the process conditions may even reach the supercritical region of water. The simulator has to cope also with this situation without loosing the accuracy of the results, or the stability of the calculation.

In power plant operation, the non-condensable gases affect the behaviour of the unit operations, such as condensers. Accurate modelling has to incorporate also this feature in the system. Also there is a need to extend the simulation to cold start up situations where the water and steam circuits initially may be filled with gas.

The challenge of global warming has lead to different technology proposals to capture carbon dioxide from the fossil fuel power plants, and storing it e.g. to geological formations. The carbon capture and storage (CCS) concepts require that the flue gas circuits may contain carbon dioxide as liquid.

The oxy fuel concepts refer to technology where pure oxygen mixed with circulated flue gases is used for burning instead of air, producing maximum carbon dioxide fraction in flue gas. Accordingly, such a power production process requires a step of separation the oxygen from air. From simulation point of view, the air related material properties must be extended to include liquid nitrogen and oxygen.

This paper discusses the implementation of these extensions in the material properties calculation, and gives illustrating modelling examples.

2 Fast material property calculation

2.1 General principles

The mostly used methods to solve pressure-flow networks in APROS are so called three equation model and six equation model. In many cases the first mentioned can be used, meaning that liquid and gas are handled in flow branches as homogeneous mixture, and both phases have the same flow velocity. However, in fast transients, such as start up of heat recovery boilers, and when studying consequences of pipe ruptures, the non-equilibrium six equation model has to be used. In this model steam and water can have different temperatures as well as different velocities. The six equation model may be used in the whole water and steam circuit, including the turbine sections. Dependable material properties calculation is needed in applications of both the homogeneous three equation thermal hydraulics model, and the non-equilibrium six equation model.

The flow circuits of the plant are spatially discretized to control volumes to enhance the mathematical solution. A fluid section module specifies the components that the fluid contains, and the way to solve material properties for thermal hydraulic nodes. Typical sections are accordingly the water and steam (WS) section, as well as the flue gas (FG) section. The material properties calculation of each section is assigned to a separate subroutine. Dynamic linking of these subroutines is provided for, which enables the users to include custom set of substances and custom material property subroutines, if required. The DLL subroutines may be programmed in either FORTRAN or C code.

2.2 Implementation aspects

Traditionally material property calculation has been very time consuming. To support real time applications the provision has been made to run material property calculation separately on parallel cores on modern processors. Both algorithms and data organization are important for achieving the required speed. In APROS version 5.9 the parallel cores of modern processors are made use of to speed up the material property calculation. The key issue for successful software implementation is to allocate frequently used data to the cache memory on chip in order to avoid the use of relatively slow main memory. It is therefore obvious that possible iteration needed in the flash calculation should be kept local.

New and wider material property functions are necessary for the modelling of the novel power plant processes. The air and CO2 separation processes e.g. require properties of liquid air, N2, O2 and CO2. During the years 2009 and 2010 new property packages of these substances have been added to the simulation platform. The implementation of the new property tables is realized via the modified EP material property section of APROS. The calculations of the EP section are performed in a DLL module (apep.dll), which includes the following substances and mixtures: Water and steam (H2O), Air, H2O + Air, Ash + Air, H2O + NaCl, Carbon dioxide (CO2), Nitrogen (N2), Oxygen (O2).

During the testing of the new fluid sections it was found that some modifications were also necessary to enhance the calculation of the process components. Thus the development effort also increased the accuracy of the process component models.

For accurate modelling of complex processes, it is required that the calculation method produces the wanted thermodynamic quantities with the given accuracy over wide range of the input arguments. In addition, very fast calculation of the properties is required, for instance in operator training simulators. This practically prevents the use of ordinary commercially existing material property databanks. Also, modification of data available in literature is typically necessary before the use for the material property calculations in the simulation platform. For example, APROS needs the properties as a function of pressure and enthalpies. To promote numerical stability in simulation applications, it is essential that the calculated values are continuous.

In this case the implementation method for the calculation the properties of air was linear interpolation with constant tabulation intervals for pressure and varying intervals for enthalpy. An alternative approach for using lookup tables is the utilization of exponential approximation functions. The functions have, however, some disadvantages due to the very high order required of the functions for large regions, discontinuities at boundaries between functions, and time consuming calculation. A novel method was developed where neural networks were used in modelling of thermodynamic properties [3]. The benefit was the straightforward implementation. Instead of typically many iteration steps, which are needed with lookup tables, the trained neural networks solve the properties by a single function call. During the recent years, the accuracy requirements for simulation have increased, also increasing the dimensions of the neural network structures. Accordingly, the approach has lost part of its practicality and attractiveness. Currently in APROS, the neural network models are used, but only for fast search of initial values. The final accuracy is guaranteed with the traditional lookup tables.

3 Non-equilibrium six equation models

As mentioned earlier, many fast transients require the use of the non-equilibrium six equation model. After the recent development, also the effects of noncondensable gases are included in the solution. The steam tables that were extended to the supercritical region are also in use.

3.1 Noncondensable gases

In the present model, it is assumed that there is only one non-condensable gas present in the simulated system, but the user can choose between four different gases: air, nitrogen, helium and hydrogen. For each gas the necessary material properties are calculated as a function of temperature. The gas density is calculated using the ideal gas equation.

The non-condensable gas can be either a part of the gas phase, or it can be as a dissolved component in the liquid phase depending on prevailing conditions. In the gas phase the non-condensable gas and the steam form a homogeneous mixture, i.e. they have the same temperature and the same velocity. The non-condensable gas distribution in gas phase is solved after the pressures, velocities and void fractions have been solved.

The dissolved gas feature of the six equation model calculates the maximum concentration of the dissolved gas as a function of pressure and temperature. On the basis of the maximum and the prevailing real concentration, the model calculates the released gas flow. This released gas is then taken into account in the gas phase solution, and in the concentration solution of the dissolved gas. If the maximum concentration is larger than the real concentration, and the gas phase has an excess of non-condensable gas, a small gas flow from gas phase to liquid is calculated, thus the gas is gradually dissolved.

Description of the non-condensable gas model, its validation, and a sample application is shown in [4].

3.2 Supercritical pressure region

At supercritical pressures the distinction between the liquid and gas phases disappears: boiling and condensation are not observed, but instead the properties of the fluid vary smoothly from those of a liquid-like fluid to those of a gas-like fluid. From macroscopic point of view, the supercritical pressure fluid can always be considered a single-phase fluid. Because of this, the homogeneous model would be ideal for the thermal hydraulic simulation at and above the critical pressure. However, in power plant applications the homogeneous model is not always sufficient for the calculation of two-phase flow below the critical pressure, and thus the six equation model has to be used.

When the six equation model is applied to supercritical pressure calculation, the problems how the model behaves near and above the critical pressure, and how the phase transition through the supercritical pressure region is handled, are inevitably encountered. Above the critical pressure, the heat of evaporation disappears and the whole concept of phase change is no longer meaningful. The set of constitutive equations needed in the six-equation solution includes friction and heat transfer correlations, which are developed separately for both phases. The capability of constitutive equations and the way how they are used has to be carefully examined. One approach, like in APROS six equation

model, to maintain separate liquid and gas flows in the numeric model, is to use a small evaporation heat and apply the concept of the pseudo-critical line. The pseudo-critical line is an extension of the saturation curve to the supercritical pressure region: it starts from the point where the saturation curve ends (the critical point), and it can be thought to approximately divide the supercritical pressure region to sub-regions of pseudo-liquid and pseudo-gas, i.e. at the same point where heat capacity is maximized, the density gradient as function of temperature is also the steepest. The thermo physical properties of water/steam undergo rapid changes near the pseudo-critical line and therefore the quality and accuracy of the steam tables is essential in calculation of flows under supercritical conditions. The steam tables used in APROS are based on the IAPWS-IF97 recommendation, which defines the properties of water with a sufficient accuracy over a wide range of parameters, including supercritical pressures. In the reference [5] the use of the six equation thermal-hydraulic model for supercritical pressure calculation is described.

4 Homogeneous three equation models

When making use of the homogeneous three equation thermal hydraulic model, the equilibrium flash calculation for the whole control volume is made in the relevant material properties subroutine. In the calculation of the air and flue gases sections the three equation model is used. Hence it is supposed that the temperatures of both phases in the control volume are the same. Also, it is assumed that the flow velocities of all phases and substances are the same. If phase separation is taking place in control volume, also the level of the liquid phase is calculated depending on the geometry of the volume. Splitting coefficients based on liquid level or other mechanisms are available for calculation of the mass fractions and energy of the flows leaving the control volume.

In each homogeneous control volume temperature of the mixture, the void fraction as well as density, specific heat capacities, dynamic viscosities and thermal conductivities of the separate phases are defined as functions of pressure, specific enthalpy of mixture and relevant mass fractions.

The next chapters show examples, how to use the new features in the modelling of processes in the oxyfuel power plants. In the oxy fuel power plants, the oxygen production is often realized by the liquefaction of air. Therefore the modelling of air separation units requires management of the thermo physical properties of air and its components from the liquid to gaseous state. On the other hand, modelling of the CCS concepts require that the carbon dioxide is liquefied. Summaries of the used properties and the basic structures of the air and carbon dioxide separation systems are presented in Fig. 1. The curves present how the saturation densities of nitrogen, air, oxygen and carbon dioxide locate in the temperature field. The presented values are based on the data of the references [6, 7, 8].

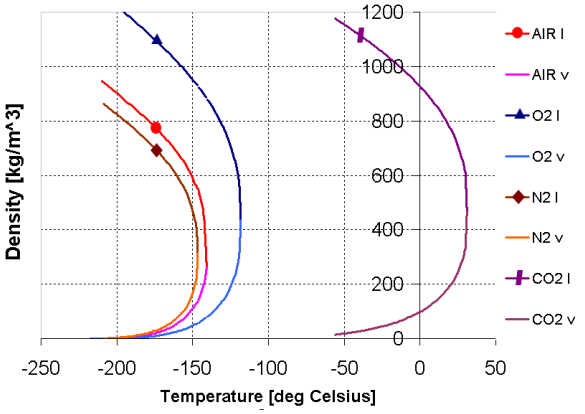

Fig. 1 Saturation densities of nitrogen, air, oxygen and carbon dioxide.

4.1 Liquefaction of air

Fig. 2 shows how the liquefaction of air process can be modelled making use of the developed features. The process consists of a compressor, a water cooler, a counter current heat exchanger, an expansion valve, and a separation tank. Air is compressed from 20 bar to 200 bar in the compressor, and cooled in the water cooler near to the available cooling water temperature. The pre-cooled air is then fed into the heat exchanger, further cooled down and expanded in the expansion valve to the liquefaction temperature. In the separation tank the gaseous and liquid contents of the air are separated. The yield of the liquid air flows out of the separation tank via the outlet valve, which controls the level of the tank. The gaseous air from the separation tank is then warmed up again in the heat exchanger and fed into the suction side of the compressor. The liquefied air is replaced by ambient air via the inlet valve.

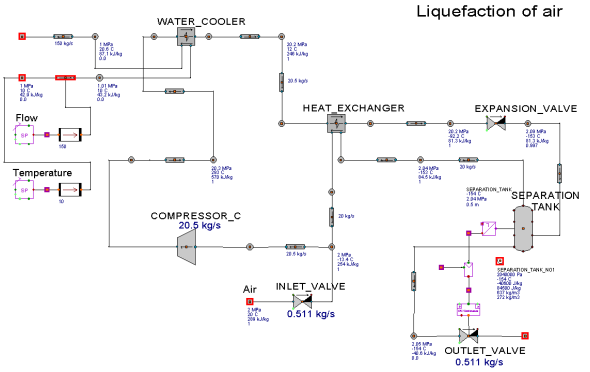

Fig. 2 Process model for the liquefaction of air.

Fig. 3 presents a simulation example. In the first modification the cooling water temperature is step wise increased by 5 degrees. Secondly, position of the expansion valve is decreased by 0.5 %. According to the first experiment, the flow of the liquid air goes down by 50 %. In the second case, the amount of the liquid air increases, when the pressure drop across the expansion valve was increased by closing the valve.

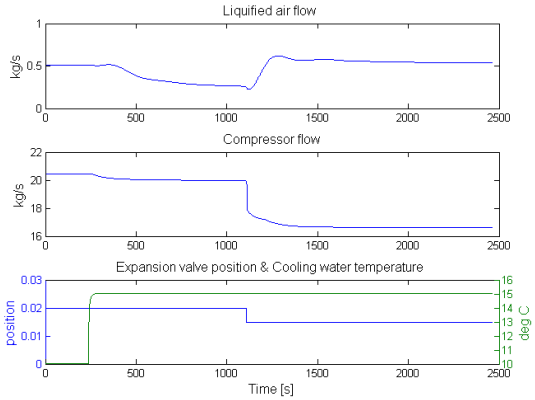

Fig. 3 Simulation experiment with the air liquefaction model.

4.2 Liquefaction of CO_2

In oxy fuel power production the flue gas consists mainly of CO_2 and water. Water is separated, and the CO_2 is liquefied for transportation. Fig. 4 presents a sample process model, which uses the extended properties of carbon dioxide for the simulation of the liquefaction process. The basic process components are used to cool down the flue gas using the refluxes from the separator tanks. In the presented process the input flows "inlet_1" and "inlet_2" go through a series of heat exchangers, which are cooled with the return flows from the two separator tanks. The expansion valves "co21_bv01" and "co21_bv02" are used for the temperature decrease by the flashing of CO_2. Finally the reverse flows "outlet_1", "outlet_2" and "outlet_3" go out from the process in the gaseous form.

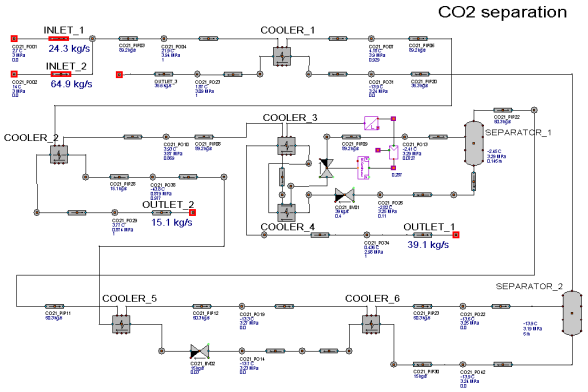

Fig. 4 Example process model for CO_2 separation.

5 Conclusions

In the presented work, accurate, fast and stable material property calculation was achieved for dynamic simulation of novel power process concepts such as the utilization of elevated (supercritical) temperature and pressure, oxy fuel combustion, and carbon dioxide capturing. Improvements in the simulation of non-condensable gases were reported too. The extended material properties and improved modelling accuracy provide a solid basis for a wide range of different simulation application fields including design evaluation, presumed disturbances analysis, commissioning planning, and operator training. The achieved speed of the rigorous calculation prepares even the way for dynamic model based factory testing of the future plant control system, in all operational conditions. Separate codes and models for each purpose are not necessarily needed. Faster commissioning times and cost savings can thus be expected whence integrating dependable simulation with the design process.

6 References

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