

CFD-Aspen Plus interconnection method. Improving thermodynamic modelling in computational fluid dynamic simulations.

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Abstract

Thermodynamic modelling in CFD is basically limited to the models available in the simulators. The method presented in this paper connects CFD simulators with Aspen Plus which instantaneously calculates and returns the value of any physical property required. Therefore, all the thermodynamic models and compounds available in Aspen Plus can be implemented in CFD simulations. The connection, created via Matlab and Excel-VBA, has been validated solving two identical CFD simulations first selecting a thermodynamic model available in the simulator and then connecting the simulator with Aspen Plus and selecting the same model. The maximum absolute average deviation between the density and viscosity values obtained in both simulations, for the two case studies analyzed, is lower than 0.7% which demonstrates the proper interconnection. The accuracy of the results obtained modeling multicomponent mixtures and supercritical fluids proves the applicability of the method to any scenarios.

Keywords: CAPE, Multicomponent Mixture, Supercritical Fluid, Pseudocomponents.

1. Introduction

Computational Fluid Dynamics (CFD) is a computer aided technique which has been extensively applied in the modelling of complex fluid flow simulations when a high degree of precision is required. Its calculation philosophy is based on the division of the model of a real piece in several cells. Then, differential equations are applied to each cell in order to obtain the evolution of both the physical properties, such as the temperature and the pressure and the flow variables, such as the velocity and the turbulence. Its precision relies on the number and on the detail of the equations solved when compared with traditional calculation methods which consider the piece as a sole control volume and apply only one equation per each unknown variable (Andersson et al., 2012).

Traditionally, CFD simulation techniques have been directly associated with fluid engineering since the development of the technology has been always linked to this discipline. Therefore, CFD techniques have been extensively applied in industries such as aerospace, aeronautic, automobile and maritime. As a consequence of this direct relationship between CFD and fluid engineering, this technique has been always linked to common fluids such as air and water and operating conditions near ideality. Consequently, the majority of the work developed in the field of CFD has been aimed at improving the flow models. Because of the high potential of this technique in applications related with chemical and process engineering, it is clearly becoming more relevant and expanding to new application fields. Nevertheless, there is still a necessity of improving the definition of the physical properties in CFD simulations in order to adequate them to uncommon compounds and mixtures and to operating conditions far from ideality. Although traditional CFD simulators allow implementing additional property methods via user defined subroutines(ANSYS, 2013a), the complexity and cost inefficiency of the process demand an alternative.

CFD research in chemical engineering is currently focused on two separate fields, the design of the base equipment where innovative and bio-based processes will be carried out and the improvement of traditional chemical engineering equipment in order to

increase the efficiency of production processes. In both cases, simulations are limited by the calculation of the physical properties. Since an accurate modelling of the physical properties requires creating and implementing in the CFD simulator complex user defined subroutines, the most common approach adopted has been to consider that the values of the physical properties remain constant (Housley et al., 2016; Kazemzadeh et al., 2016; Kim et al., 2016; Klenov et al., 2015; Luo et al., 2016; Nguyen et al., 2012; Troshko and Zdravistch, 2009). This is an acceptable approach in the case of single components and almost isothermal processes. However, when the complexity increases, for example in the case of processes with high temperature gradients, this approach is not correct. In these cases, the physical properties have been sometimes modelled applying polynomial functions of the temperature (Maffei et al., 2016; Saeed et al., 2016), the kinetic gas theory (Wehinger et al., 2016) or considering the ideal gas law (Wang et al., 2009; Wu et al., 2010). Only in a very limited number of examples, more detailed models such as the Peng Robinson equation have been considered (Amrei et al., 2014). In the case of multicomponent simulations, commonly, simple mixing laws have been implemented (Stefanidis et al., 2006).

Consequently, the challenge linked to chemical engineering CFD simulations is to obtain an accurate modelling of the physical properties in conditions either of ideality or of non-ideality from any set of pressure, temperature and composition (values which characterize any system) (ANSYS, 2013b). Therefore, it is clearly necessary to develop an alternative to the creation of user defined subroutines which contain the desired thermodynamic models because of the complexity and time required in the process.

One of the most extended chemical engineering simulators is the commercial software Aspen Plus® of the company AspenTech®. It is commonly used both in the simulation of real processes and in the design of grass roots new ones. The success of this simulator has been based on its extensive available database of compounds and thermodynamic models which have been developed during its 35 years of existence. With this database, it is possible to simulate almost any type of compound and mixture in the majority of operating conditions.

In this paper an innovative method which connects CFD simulators with Aspen Plus® is presented. Therefore, anytime that the CFD simulator requires the value of a physical property, it activates Aspen Plus® sending the corresponding set of pressure,

temperature and composition values. Then, Aspen Plus® calculates the value of the demanded physical property using the desired thermodynamic method which has been previously selected. Finally the physical property value is returned to the CFD simulation which continues calculating the solution. When an additional physical property value is required, the process is repeated. Consequently, the accuracy of CFD simulations is increased resulting in a better modelling of the flow behavior. Furthermore, the extensive compounds database of Aspen Plus® allows creating any new compound in the CFD simulator regardless whether it is already available in its own database.

2. Description of the method

The objective of this paper is to present a method which allows connecting CFD software with Aspen Plus®. Thus, all the compounds and thermodynamic packages available in Aspen Plus® can be implemented in CFD simulations.

Ansys Fluent® is the base CFD software selected to validate the method. This commercial CFD simulator allows customizing its simulations via “C” language subroutines. Focusing on the physical properties modelling, anytime that the physical properties methods available in Ansys Fluent® are not precise enough, the alternative methods must be programmed in a “C” language subroutine which is implemented in the simulation. The complexity of programming a complete property method and the necessity of testing the subroutine before its application in the CFD simulation in order to find possible mistakes is not cost effective. For this reason a new method which directly connects Ansys Fluent® with Aspen Plus® has been created. Instead of programming complex “C” language subroutines, the user can directly select the compounds and thermodynamic packages desired in Aspen Plus®. Then, while the CFD simulation is being run, anytime that a physical property value is required, the CFD software automatically runs with the required values of pressure, temperature and composition the corresponding Aspen Plus® simulation where the desired compounds and property packages have been selected, returning the corresponding physical properties values.

As it was previously explained in this section, the only customization method allowed by Ansys Fluent® is the implementation of “C” language subroutines. Therefore the

starting point in the method of connection of Ansys Fluent® and Aspen Plus® must be a “C” language subroutine. The objective of this subroutine is to obtain the required values of pressure, temperature and composition and send them to Aspen Plus® in order to calculate physical properties such as the density, the specific heat, the thermal conductivity and the viscosity.

On the other side of the connection, one of the most extended methods used to customize Aspen Plus® is via Excel® VBA (Visual Basic for Applications) (AspenTech, 2014). Commonly, a set of required characteristic variables of a unit operation are extracted from Aspen Plus®, implemented in a mathematical model programmed in VBA and the corresponding result is sent back to Aspen Plus®. When the complexity of the mathematical model requires a more powerful mathematical tool than Excel VBA, the model is programmed in a more specific mathematical software such as Matlab®. Then, Excel VBA is used only as the nexus between Aspen Plus® and Matlab®(Matlab, 2015). This option has been the one explored, developed in this method and presented in this paper.

Therefore, the “C” language subroutine must be able to exchange information between Ansys Fluent® and Matlab®. This subroutine is activated when required by Ansys Fluent® to send values of pressure, temperature and composition and to receive the corresponding values of density, specific heat, thermal conductivity and viscosity. One of the advantages of using Matlab® as nexus is the possibility of checking the evolution of the calculations performed by Aspen Plus® since the physical property values are stored in Matlab®.

It is stated here that although Matlab® and Excel® VBA are used in this method as nexus between Ansys Fluent® and Aspen Plus®, both programs can be directly connected with the CFD simulator. For instance, an available possibility to reduce the computational time when the CFD simulation requires the value of many unknown physical properties values is the creation of a Matlab® array which contains all the required values (Aspen Plus® can be directly run from Matlab® to simplify the creation of the array). This array is directly and almost instantaneously read by Ansys Fluent® at the beginning of each simulation limiting the number of connections with Aspen Plus® only to the calculation of additional values which are not included in the array.

Although the method presented in this paper is focused on the use of Ansys Fluent® since it is one of the most extended CFD simulators, the implementation of the method

to other CFD simulators is not restricted. To authors' knowledge, the majority of CFD simulators allow the implementation of user defined subroutines to customize their CFD simulations as it is the case of the User Defined Functions written in "C" language in Ansys Fluent®. The basic difference between the available simulators is the computer language used in the definition of the code. For example, while in the case of Ansys CFX®, the computer code shall be programmed in "Fortran", in Comsol® the code shall be written in Matlab® language. Open Foam® allows the implementation of functions via "C++" language code. Finally, in the case of Star-CCM+ the computer code can be written in "C", "C++" or "Fortran" language. The possibility of implementing user defined subroutines in different CFD software allows expanding the execution of the method presented in this paper to all these other simulators. The only requirement is the creation of a subroutine written in the computer language allowed by each CFD simulator in order to be able to exchange information with Matlab®.

A scheme of the interconnection method between Ansys Fluent® and Aspen Plus® presented in this section is shown in Figure 1:

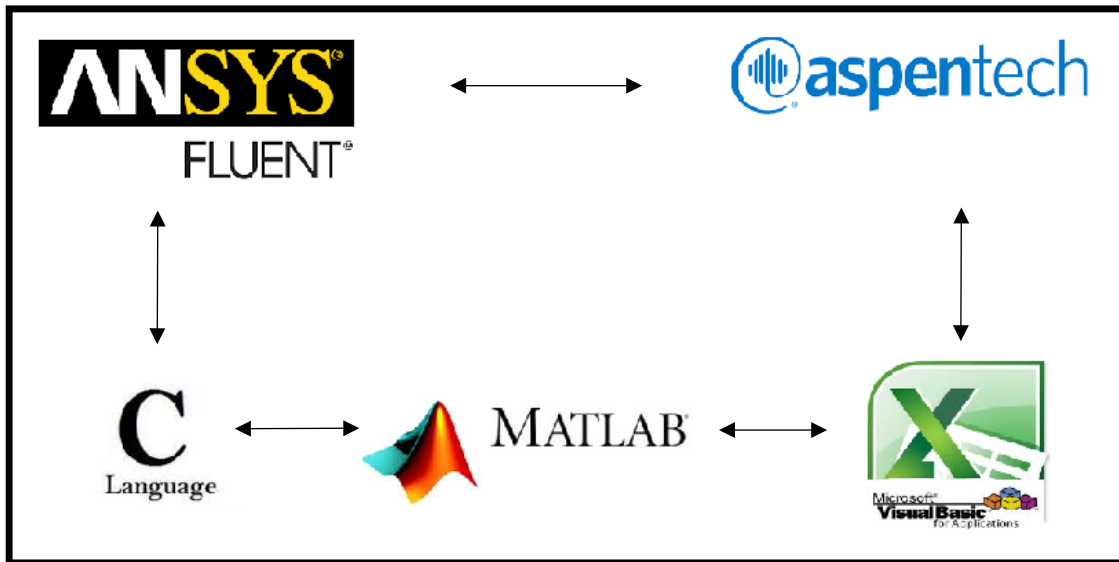


Fig. 1. Method of connection of Ansys Fluent® and Aspen Plus®.

Figure 1 shows the method of connection **between** Ansys Fluent® **and** Aspen Plus®. From an operational point of view, the first step is to select the desired compounds and thermodynamic method in an Aspen Plus® simulation. An additional option is the creation of a thermodynamic model from experimental data via Aspen Properties® which can be easily implemented in an Aspen Plus® simulation. This process allows

calculating physical properties directly from models created from experimental data. Then, when the CFD simulation is being run and anytime that Ansys Fluent® requires the value of a physical property; it sends the pressure, temperature and composition of the corresponding cells to Matlab® via the “C” language subroutine. These values are stored in matrices in Matlab® and they are transferred to Aspen Plus® via Excel® VBA. Aspen Plus® calculates the values of the required physical properties which are sent back to Matlab® via Excel® VBA. Finally the values of the physical properties, which are again stored in matrices, are sent back to Ansys Fluent® via the “C” language subroutine and implemented in the CFD simulation. Anytime that Ansys Fluent® requires a physical property value, the process is repeated. When the simulation ends, all the calculated values can be checked on Matlab®. A more detailed explanation of the working principles of the method can be found in the Appendix 1 of this paper.

In multiphase CFD simulations, slight modifications in the method are required. First, in the case of multicomponent fluids, although a set of pressure, temperature and composition values determines the vapor fraction, special care has to be taken in order to read from Aspen Plus® the physical properties which correspond with the phase demanded by Ansys Fluent®. The addition of a flash vessel to the Aspen Plus® simulation facilitates this selection. In case that the vapor phase properties are required, the physical properties of the upper outlet stream of the flash shall be read. On the other hand, if the liquid properties are required, the physical properties of the lower outlet stream of the flash shall be selected. Regarding pure components, in addition to the pressure and the temperature, the vapor fraction of the different cells shall be read. If the value of this parameter is between 0 and 1, two phases are present in the cell. In these cases, in the “C” algorithm which demands the properties of the vapor phase to Aspen Plus®, the temperature shall be substituted by the vapor fraction whose value in this case is equal to 1, and in the algorithm which demands the properties of the liquid phase to Aspen Plus®, the temperature shall be substituted by the vapor fraction whose value in this case is equal to 0.

When a user defined subroutine is implemented in a CFD simulation, a key parameter which has to be considered is the computational time. As it is explained in the Appendix 1, the method of connection allows the user to select the required accuracy of the thermodynamic properties values. This is directly controlled modifying the tolerances which represent the acceptable margins in pressure, temperature and composition used

in further interpolations of physical property values using the ones which have been already calculated. For example, if it is required to model the density evolution in an atmospheric water mixer in which two streams at 30°C and 60°C are mixed, the user can select 5°C as an acceptable limit of temperature tolerance. This means that the user considers that there are not strong variations in the density in intervals below 5°C in this temperature and pressure ranges. The subroutine will calculate the density each 5°C and will interpolate the rest of the required values. If the tolerance is reduced to 1°C, the accuracy is increased since the interpolation is performed **within** lower ranges.

Nevertheless, the number of values which have to be calculated is multiplied by a factor of five increasing the calculation time by the same factor. **The authors have quantified that the time required per calculation, which is the time required to calculate one physical property value, in a personal computer with 32GB of RAM memory and an Intel® Core™ i7-4770 processor, is equal to 7.3s when the method is computed in serial.** In this example, if it is considered that 5°C is a reasonable margin to calculate the density due to the smooth variations in this temperature range, as the temperature difference is equal to 30°C, only seven values shall be calculated by Aspen Plus® and therefore, the total calculation time required would be increased by 51.1s. When more than one physical property is required, the method calculates the different physical properties in parallel (opening at the same time different Aspen Plus® simulations) and the global calculation time is equal to the calculation time of the physical property which requires a higher number of values (7.3s multiplied by the number of values required by the physical property **which determines the calculation time**). Since the method stores the calculated values in “C” matrices, in the following CFD iterations Ansys Fluent® only reads or interpolates the values avoiding recalculations from Aspen Plus®. Both the reading of the stored values and the interpolation between these values are almost instantaneous processes which do not increase the global calculation time.

Moreover, it is important to point out, especially in the case of multicomponent simulations, that the subroutine does not calculate the values of the physical properties required for all the possible combinations of pressure, temperature and composition. The method calculates only those values demanded by Ansys Fluent®. This considerably reduces the calculation time.

Regarding to the influence of the subroutine in the global convergence of the CFD simulation, the authors have verified that this method does not produce any disturbance in this parameter as shown later in the validation examples.

Finally, the parallelization options of this method have been analyzed. The base method presented in this paper has been programmed to be run in serial and this option is the only one which is currently available. Nevertheless, the authors have checked that the method will be able to run in parallel whether the current connections between the “C” language subroutine and Matlab®, Matlab® and Excel VBA and Excel VBA and Aspen Plus® are modified to be executed in parallel.

3. Results and discussion

The validation of the CFD-Aspen Plus® interconnection method, whose fundamentals have been explained in the second section of this paper, has been carried out running two different case studies. In each case study, two CFD simulations have been calculated and compared. First, the simulation has been solved selecting one of the thermodynamic methods available in Ansys Fluent® and then, the simulation has been executed again but activating the CFD-Aspen Plus® connection method and selecting the same thermodynamic method in Aspen Plus®. Once that both simulations have been solved, a physical property has been selected as a basis of comparison and the absolute average errors between the results obtained in both simulations have been calculated. Later, the applicability of the subroutine to more complex scenarios such as a multicomponent mixture and a supercritical fluid is demonstrated.

The mathematical equation selected to compute the absolute average errors between the values obtained from both simulations is shown in equation (1):

$$err(\%) = \frac{|(calculated\ value - theoretical\ value)|}{theoretical\ value} \cdot 100 \quad (1)$$

The calculated value is the physical property value obtained from the simulation in which the interconnection method is implemented. On the other hand, the theoretical

value has to be understood as the value obtained when a physical property method available in Ansys Fluent® is selected or as the theoretical value used as basis of comparison.

It is remarked here, that the objective of this interconnection method is not to replace the phase calculation models available in CFD simulators but to provide values of physical properties requested by the CFD simulator to Aspen Plus®. This is especially relevant and it has to be understood in the case of liquid-vapor CFD simulations. In these cases, commonly either the Lagrangian or the Eulerian approaches are chosen. This interconnection method does not substitute any of these approaches. This means that in the resolution of these CFD simulations, one of these approaches has to be selected but, when the physical properties are required, Ansys Fluent® activates Aspen Plus® and the required values are provided. For example, in a liquid-vapor CFD simulation, the user can decide to select the Eulerian-Eulerian approach and at the same time implement this connection method in order to calculate the density of the liquid phase using the NRTL method while the density of the vapor phase is calculated by the Soave Redlich Kwong Equation.

A simple mixer, similar to a “T” type one, has been selected as the base geometry to solve the CFD simulations. While the diameter of its two inlets is equal to 55mm, the diameter of its outlet is equal to 78mm. An unstructured tetrahedral 3D mesh of 55000 elements shown in Figure 2 has been generated. Since the objective of the CFD simulations is only to prove the applicability of the method, neither mesh refining studies nor mesh independence tests have been performed.

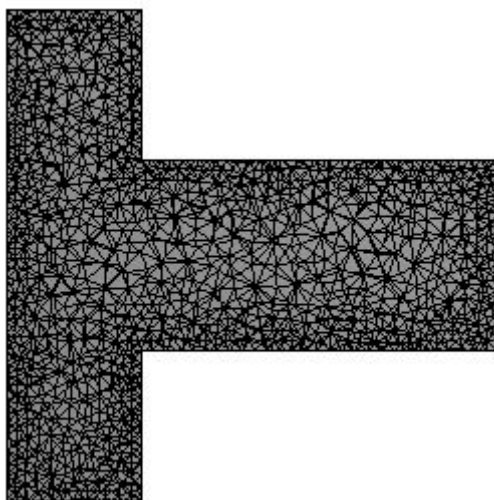


Fig. 2. Tetrahedral 3D mesh generated and implemented in the CFD simulations presented in this paper.

3.1 First validation example

The first validation example is basically the mixture of two liquid water streams at different temperatures and at atmospheric pressure.

Two water streams of 3 kg/s, the first one at 20°C and the second one at 90°C, are mixed. In the first simulation, the NIST real gas method included in Ansys Fluent® has been selected. This method is based on water property tables developed by the National Institute of Standards and Technology. On the other hand, in the second simulation the IAPWS water method has been selected in Aspen Plus®. This method is based on water property tables developed by the International Association for the Properties of Water and Steam. Both methods present almost identical results.

In this first validation example, the viscosity is the physical property selected as basis of comparison because of its appreciable variations in this temperature range. Moreover, it is considered that because of the almost negligible pressure drop, in this example the physical properties are only influenced by the temperature.

In order to numerically quantify the discrepancies between the viscosity values from both simulations, viscosity results are reported and compared from 20°C to 90°C each 10°C in Table 1:

| Temperature (°C) | Viscosity, Theoretical Value (kg/m·s) | Viscosity, Calculated Value (kg/m·s) | Absolute Average Deviation (%) |
|------------------|---------------------------------------|--------------------------------------|--------------------------------|
| 20,0 | 9,95E-04 | 9,99E-04 | 0,45 |
| 30,0 | 8,00E-04 | 7,99E-04 | 0,06 |
| 40,0 | 6,57E-04 | 6,59E-04 | 0,18 |
| 50,0 | 5,53E-04 | 5,53E-04 | 0,00 |
| 60,0 | 4,73E-04 | 4,74E-04 | 0,26 |
| 70,0 | 4,11E-04 | 4,12E-04 | 0,21 |
| 80,6 | 3,61E-04 | 3,62E-04 | 0,08 |
| 90,0 | 3,21E-04 | 3,21E-04 | 0,00 |

Table 1. Numerical comparison of the viscosity values obtained selecting the NIST real gas method in Ansys Fluent® (theoretical value) and interconnecting Ansys Fluent® with Aspen Plus® and selecting the IAPWS water method in Aspen Plus® (calculated value).

A good agreement between the results obtained in the first simulation in which the NIST real gas method is selected and in the second simulation in which Ansys Fluent® is interconnected with Aspen Plus® selecting the IAPWS steam tables is clearly observed. Since the maximum absolute average deviation is lower than 0.5%, it is considered that Ansys Fluent® is properly connected with Aspen Plus® and therefore the method is validated.

3.2 Second validation example

An additional validation example to the one presented in subsection 3.1 is analyzed hereafter.

In this case, two air streams, the first one at 50°C and the second one at 250°C are mixed. Both the inlet pressure and the mixer pressure drop are fixed at 1.01 bara and 0.01bar. Therefore, as in the previous example, it can be considered that the physical properties are only influenced by the temperature variations. In this case, the density is the physical property used as basis of comparison. First, the simulation is solved selecting the Peng Robinson equation, available in Ansys Fluent®, to calculate the density values. Then Ansys Fluent® is interconnected with Aspen Plus® and the Peng Robinson equation is selected in Aspen Plus®.

In order to numerically quantify the discrepancies between the density values from both simulations, the density results are reported and compared from 50°C to 250°C each 20°C in Table 2:

| Temperature (°C) | Theoretical Value (kg/m ³) | Calculated Value (kg/m ³) | Average Deviation (%) |
|---------------------|---|--|--------------------------|
| 50,00 | 1,100 | 1,102 | 0,11 |
| 70,00 | 1,031 | 1,024 | 0,66 |
| 90,00 | 0,973 | 0,972 | 0,07 |
| 110,00 | 0,922 | 0,925 | 0,30 |
| 130,00 | 0,883 | 0,877 | 0,66 |
| 150,00 | 0,839 | 0,837 | 0,21 |
| 170,00 | 0,797 | 0,800 | 0,30 |
| 190,00 | 0,764 | 0,767 | 0,34 |
| 210,00 | 0,734 | 0,738 | 0,55 |
| 230,00 | 0,698 | 0,703 | 0,68 |
| 250,00 | 0,679 | 0,680 | 0,12 |

Table 2. Numerical comparison of the density values obtained selecting the Peng Robinson equation in Ansys Fluent® (theoretical value) and interconnecting Ansys Fluent® with Aspen Plus® and selecting the Peng Robinson equation in Aspen Plus® (calculated value).

As in the previous example, the good agreement between the results obtained from both simulations validates the method. In this case, the maximum absolute average deviation is lower than 0.7%.

3.3 Multicomponent simulation

The applicability of the subroutine to a CFD simulation of a multicomponent mixture is tested in this subsection.

In this case study, two liquid streams, the first one of 3kg/s of water and methanol, $X_{\text{water}}=0.5$ w/w, and the second one of 3kg/s of ethanol and propanol, $X_{\text{ethanol}}=0.5$ w/w, are mixed. Both the pressure and the temperature remain constant at 1atm and 11°C.

In this case, because of the polarity of the liquid compounds, the NRTL thermodynamic method is selected. However since this method is not available in Ansys Fluent®, the results obtained from the CFD simulation when Ansys Fluent® is connected with Aspen Plus® selecting the NRTL method, are compared with the ones directly obtained from a simulation of Aspen Plus® in which this method is chosen.

As in the previous validation example explained in subsection 3.2, the density is the physical property used as basis of comparison. The numerical discrepancies between the

density values for mixtures of different compositions are reported and compared in

Table 3:

| xH ₂ O (w/w) | xCH ₃ OH (w/w) | xC ₂ H ₅ OH (w/w) | xC ₃ H ₇ OH (w/w) | Density, Theoretical Value (kg/m ³) | Density, Calculated Value (kg/m ³) | Absolute Average Deviation (%) |
|----------------------------|------------------------------|--|--|---|--|--------------------------------------|
| 0,02 | 0,01 | 0,55 | 0,42 | 820,2 | 825,1 | 0,60 |
| 0,10 | 0,06 | 0,47 | 0,36 | 827,3 | 829,7 | 0,29 |
| 0,18 | 0,10 | 0,41 | 0,31 | 834,1 | 839,4 | 0,62 |
| 0,24 | 0,14 | 0,35 | 0,27 | 839,7 | 833,8 | 0,70 |
| 0,30 | 0,17 | 0,30 | 0,23 | 845,3 | 840,4 | 0,59 |
| 0,41 | 0,23 | 0,21 | 0,16 | 856,1 | 856,7 | 0,06 |
| 0,48 | 0,27 | 0,14 | 0,11 | 864,8 | 866,0 | 0,14 |
| 0,54 | 0,30 | 0,09 | 0,07 | 872,7 | 873,2 | 0,05 |

Table 3. Numerical comparison of the density values obtained from a direct simulation selecting the NRTL equation in Aspen Plus® (theoretical value) and interconnecting Ansys Fluent® with Aspen Plus® and selecting the NRTL equation in Aspen Plus® (calculated value).

As in the validation cases, Ansys Fluent® is properly connected with Aspen Plus® since the maximum absolute average deviation is equal to a 0.7%. Therefore, the applicability of the method to multicomponent CFD simulations is proven.

3.4 Supercritical fluid simulation

Finally, in this subsection the applicability of the subroutine to a CFD simulation in which a supercritical fluid is involved is tested.

In this simulation, two water streams of 3kg/s at 250bara, the first one at 20°C and the second one at 400°C are mixed. In this conditions, there is a pseudocritical point between 380°C and 390°C where the specific heat increases sharply. Since the pressure remains over 250bara, the vapor phase is not generated in the mixer and therefore it can be considered that only one phase exists (pressurized liquid). Consequently neither the Lagrangian approach, in which the fluid phase is modelled as a continuum by solving the Navier-Stokes equations and the dispersed phase is modelled by means of a large number of individual particles, nor the Eulerian approach, in which the different phases are all treated as continuous phases (Andersson et al., 2012), are implemented. It is noted that the main objective of this subsection example is to demonstrate the ability of the

method in the calculation of the physical properties even in the vicinities of the critical point.

Although in the first validation example presented in subsection 3.1 the NIST real gas model was selected in Ansys Fluent®, it has been tested that this method does not accurately work in supercritical conditions. Therefore, the methodology which has been applied in subsection 3.3, this is the comparison of the results versus the ones directly obtained from a simulation in Aspen Plus®, is followed in this subsection. As in subsection 3.1, the IAPWS water and steam tables were selected in Aspen Plus® as thermodynamic model.

In this case, the enthalpy was selected as the basis of comparison. The enthalpy of water at 25°C and 1atm (-15866 kJ/kg) has been considered as reference enthalpy and it has been subtracted to all the results obtained in both simulations. The numerical discrepancies between the enthalpy values from both simulations are reported and compared from 20°C to 400°C and are presented in Table 4:

| Temperature (°C) | Enthalpy, Theoretical Value (J/kg) | Enthalpy, Calculated Value (J/kg) | Absolute Average Deviation (%) |
|------------------|------------------------------------|-----------------------------------|--------------------------------|
| 20,00 | 1,68E+03 | 1,69E+03 | 0,47 |
| 100,00 | 3,32E+05 | 3,34E+05 | 0,45 |
| 200,00 | 7,57E+05 | 7,58E+05 | 0,10 |
| 300,00 | 1,23E+06 | 1,23E+06 | 0,00 |
| 350,00 | 1,54E+06 | 1,54E+06 | 0,00 |
| 380,00 | 1,83E+06 | 1,84E+06 | 0,42 |
| 385,00 | 2,04E+06 | 2,05E+06 | 0,46 |
| 400,00 | 2,47E+06 | 2,47E+06 | 0,01 |

Table 4. Numerical comparison of the enthalpy values obtained from a direct simulation selecting the IAPWS tables in Aspen Plus® (theoretical value) and interconnecting Ansys Fluent® with Aspen Plus® and selecting the IAPWS tables in Aspen Plus® (calculated value).

As in the previous cases, Ansys Fluent® is properly connected with Aspen Plus® since the maximum absolute average deviation is lower than a 0.5%. Therefore, since the enthalpy discrepancies are lower than 1% in all the temperature range, the applicability of the method to supercritical CFD simulations is validated.

3.5 Discussion

The method of connection presented in this paper allows implementing in CFD simulations all the compounds and thermodynamic packages available in Aspen Plus®. The objective of this section is to show all the potentiality of the method proposing improvements to CFD simulations [which have been](#) already published in literature.

The first example presented here is a simulation which studied the improvement of the oven efficiency in the drying process of the can making industry (Tanthadiloke et al., 2016). In this work, an air stream evaporates ethylene glycol mono butyl ether ($C_6H_{14}O_2$), which is the solvent of the process. The physical properties of the solvent were considered constant and directly obtained from literature. As this solvent is an uncommon polar compound, an interesting alternative is to generate a suitable thermodynamic model from experimental data via Aspen Properties® and export it to Aspen Plus®. Therefore, the physical properties in the CFD simulation would be calculated directly from a model generated from experimental data increasing the accuracy of the simulation.

Another interesting example of the [applicability](#) of CFD modeling to chemical engineering, is the analysis of the pressure and temperature evolution [profiles](#) during the undesired scenario of a fire in a LPG vessel (Landucci et al., 2016). In this work, the fluid was considered as a real gas and consequently, the Peng Robinson equation was programmed and implemented via a “C” language subroutine. Although this approach is totally acceptable, it is common that in the refining and petrochemical industry some vessel could be filled with different fluids depending on the operating case (especially in batch operations). If this is the case, it would be necessary to reprogram the subroutine in order to consider the corresponding fluids in each scenario. The use of the method of interconnection allows directly selecting the desired compounds in Aspen Plus® without the necessity of rewriting the subroutine.

Regarding to multicomponent and multiphase simulations, flow modelling studies are quite often presented in literature (Padoin et al., 2014). It is reminded here again that the objective of the method of connection is not to replace neither the traditional [Eulerian-Lagrangian approach, in which the fluid phase is modelled as a continuum by solving the Navier-Stokes equations and the dispersed phase is modelled by means of a large number of individual particles, nor the Eulerian-Eulerian approach, in which the](#)

different phases are all treated as continuous phases(Andersson et al., 2012), but to provide the simulator with the required physical properties per each phase. In this work, two mixtures, the first one of water and air and the second one of methane, pentane, hexane and octane mixture are modelled. The physical properties of the vapor phase are calculated considering the fluid as an ideal gas and applying a mass weighted mixing law. When complex compounds and pressurized systems are considered, these thermodynamic models may not provide sufficiently precision in the results. Moreover, programming in a user defined subroutine more detailed mixing laws is a complex and time consuming effort. The selection in Aspen Plus® of a thermodynamic model with a more accurate mixing law would increase the accuracy of the CFD simulations.

An example of the application of CFD modeling to the refining and petrochemical industries is the study of the liquid film vaporization of a multicomponent fuel (Zhang et al., 2017). First, it is noted the reduced number of refining and petrochemical units which have been modeled in CFD. The main inconvenience in this type of simulations is the characterization of oil fractions. In process engineering, oil fractions have been traditionally characterized by means of pseudocomponents. Pseudocomponents are fictitious compounds created by process engineering simulators whose mixtures are able to accurately define oil streams. The characterization of an oil stream requires an elevated number of pseudocomponents whose creation will demand an excessive amount of time in any CFD software. Moreover, the complexity of the simulation would be increased since a *species* model would be required. In this example, the fluid presented in the work is a diesel fraction which has been characterized as a single compound with constant properties. The implementation of the method of interconnection allows easily defining the mixture as a single compound in Ansys Fluent®, characterize the oil fraction in Aspen Plus® by means of pseudocomponents and select the proper thermodynamic method, as for example, the traditional Grayson-Streed Lee-Kesler thermodynamic package used in refining simulations.

Finally, although the number of publications related with CFD modeling of supercritical fluids applications is reduced, an available example is the simulation of a transpiring wall reactor used in supercritical water oxidation(Bermejo et al., 2010). In this work, the Peng-Robinson equation of state coupled with the Magoulas-Tassios translated volume correction is implemented via a user define subroutine in order to calculate the density.

Moreover, the specific heat is calculated applying a mass weighted average law. As a consequence of the drastic variations of the specific heat of water near the critical point, calculation errors arise and therefore the solution diverges when the values of this physical property are directly interpolated from a table of experimental data. For this reason, in this work it was decided to create an apparent specific heat - temperature table with steadier interpolation slopes, maintaining the global area behind the specific heat-temperature curve in order to conserve the total enthalpy. This technique is acceptable if only the global energy balance is considered. However, when the temperature profile is required, this method does not accurately predicts the temperature variations near the critical point because of the adaptation of the specific heat values in this zone. The implementation of the method of connection (as demonstrated in section 3.4) allows accurately modelling both the specific heat and the enthalpy in any fluid region.

4. Conclusions

A method of interconnection between CFD simulators and Aspen Plus® via Matlab® and Excel-VBA has been presented in this paper. Anytime that the value of a physical property is required, the CFD simulator activates Aspen Plus®, where the desired thermodynamic method has been selected, the physical property value is calculated and it is returned to the CFD simulator. The method has been programmed to be computed in serial. Nevertheless, the parallelization of the method is allowed. The time required in the calculation of each physical property value is equal to 7.3s [with a computer of 32GB of RAM memory and an Intel® Core™ i7-4770 processor](#). However, the values calculated by Aspen Plus® are stored in matrices and later, interpolations are performed reducing the global calculation time.

The method of connection has been validated studying two different case studies. In the first one, two streams of liquid water at different temperatures are mixed. The simulation has been solved first selecting the NIST real gas thermodynamic method available in Ansys Fluent® and then, interconnecting Ansys Fluent® with Aspen Plus® selecting the IAPWS thermodynamic method in Aspen Plus® (totally comparable with the NIST real gas thermodynamic method). The viscosity values obtained in both simulations have been compared calculating the absolute average discrepancies between them. Since the maximum absolute average discrepancy is lower than 0.5%, the method is validated. In a second validation example, two air streams at different temperatures

are mixed. The validation philosophy followed has been the same than in the previous case but selecting the density as basis of comparison. In this case, the maximum absolute average discrepancy is lower than 0.7%, corroborating the validation of the model. Finally, the results obtained modeling a multicomponent mixture and a supercritical fluid (maximum absolute average discrepancy lower than 0.7%) prove the applicability of the method to the modeling of any type of fluids at any operating conditions.

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Appendix 1

In this appendix, a detailed explanation of the working principles of the method of connection of Ansys Fluent® and Aspen Plus® is presented.

It is noted that the base of the method is the connection of Ansys Fluent® and Aspen Plus® via a “C” language subroutine, Matlab® and Excel VBA. Therefore, although the subroutines explained in this section are the ones created by the authors, any additional subroutines programmed by new users of the method and able to perform these connections are equally valid.

A.1.1 “C” language subroutine

In this subsection of the appendix, the working mechanisms of the “C” subroutine which connects Ansys Fluent® with Matlab® is explained. Figure A.1 shows a scheme of the subroutine:

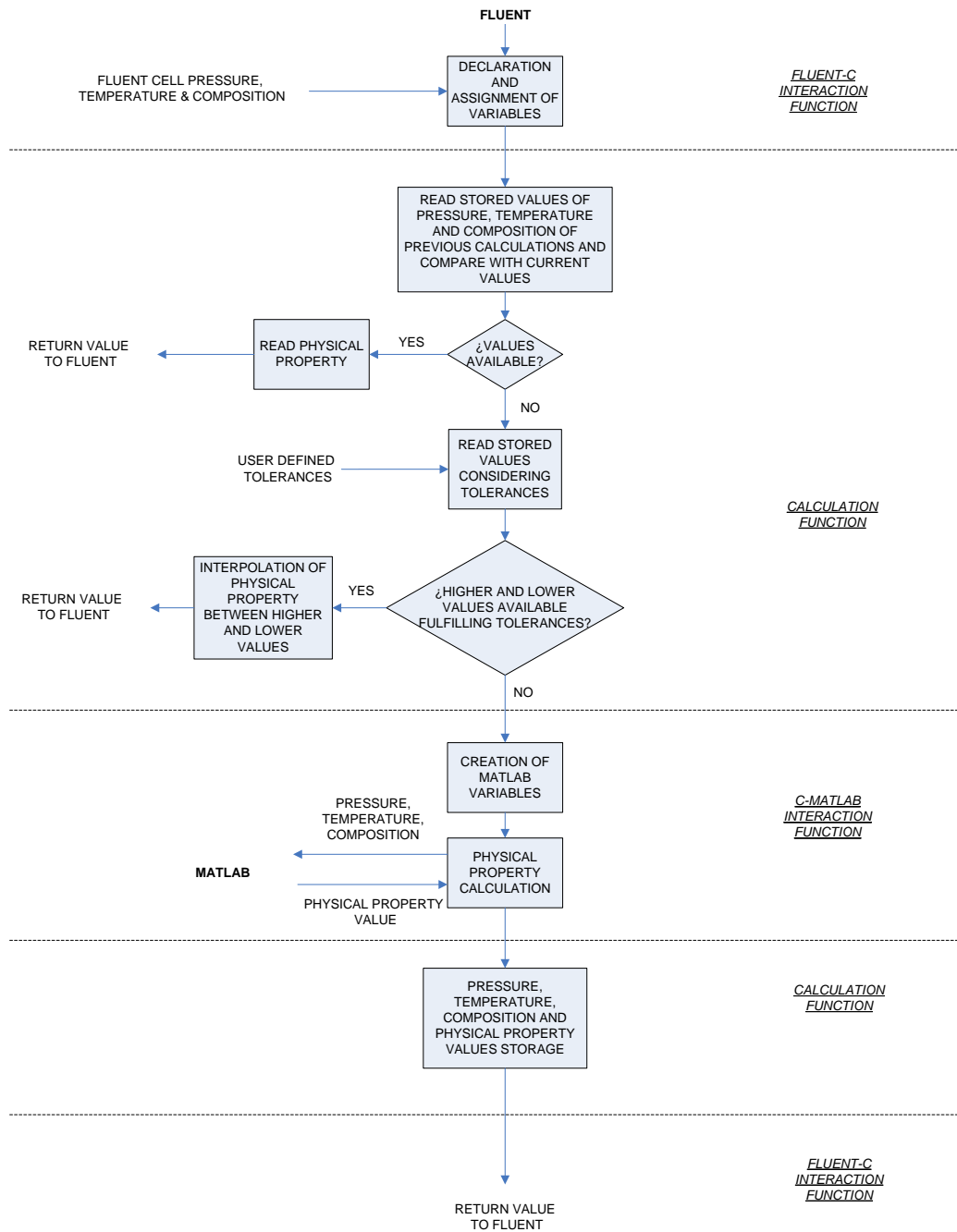


Fig.A.1. Scheme of the “C” subroutine which connects Ansys Fluent® with Matlab®.

In the first step, Fluent passes the values of the pressure, the temperature and the composition to the “C” language subroutine. These values are stored in “C” variables which are declared at the beginning of the code. The subroutine calls the calculation function passing the pressure, temperature and composition which are stored in variables declared at the beginning of this function. First, it is checked whether the desired property has been already calculated for those values of pressure, temperature and composition. In case that the physical property value is already available for these

conditions, the value is read and returned to Fluent. On the other hand, if the physical property value is not available, additional calculated values in a range defined by the user by means of tolerances are searched. For example, if the required temperature is 60°C and the selected tolerance in temperature is 10°C, any available values between 50°C and 70°C are selected. If a larger and a smaller value within the range of the tolerance are found, the required value of the physical property is interpolated. Using the data of the previous example, if values of the physical property are available for temperatures of 53°C and 65°C, the value at 60°C is interpolated using the previous values as lower and upper limits. Once that the property has been interpolated, its value is returned to Fluent. On the other hand, if there are not values which can be used in the interpolation, the “C” subroutine calls to the “C”- Matlab® connection function. This function creates Matlab® variables with the values of the temperature, pressure and composition, starts Matlab® and waits until the physical property has been calculated. Once that the value is returned, the pressure, temperature, composition and the own physical property value are stored in matrices. Finally, the value is returned to Fluent.

A.1.2 Matlab® code

In this subsection of the appendix, the Matlab® code which receives the values of the pressure, the temperature and the composition from the “C” language subroutine and transfers them to Excel® VBA is explained. Figure A.2 can be used as a reference in this subsection:

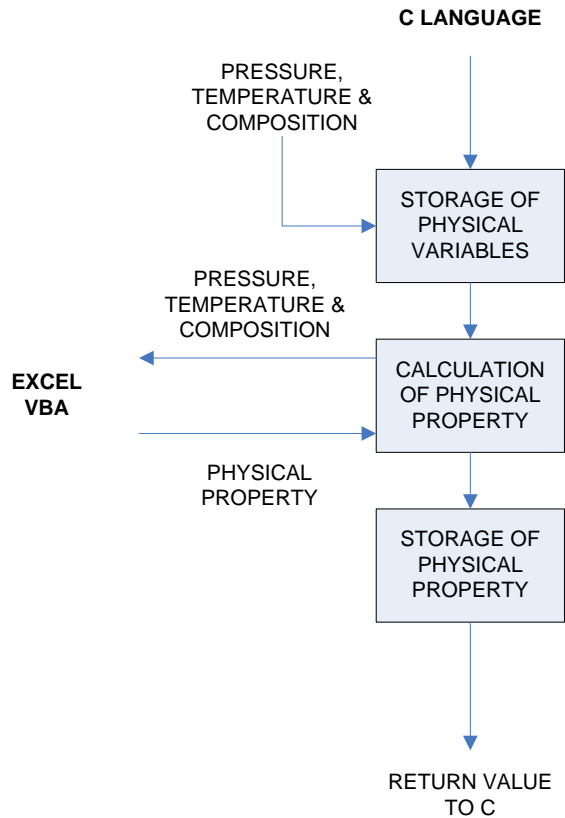


Fig.A.2. Scheme of the Matlab code which connects the “C” language subroutine with Microsoft Excel® VBA.

The values of the Matlab® variables created by the “C” language subroutine are stored in matrices. Matlab® calls Excel VBA and transfers these variables. When the physical property has been calculated and returned back to Matlab® via Excel VBA, it is stored in a matrix. It has to be noted that since the values of the temperature, pressure, composition and physical properties are stored in Matlab® matrices, it is possible to check when required all the physical property values which have been calculated during a CFD simulation. Finally, the value of the physical property is returned back to the “C” language subroutine.

A.1.3 Microsoft Excel® VBA code

In this final subsection of the Appendix, the Excel® VBA subroutine which receives the values of the pressure, temperature and composition from Matlab® and transfers them to Aspen Plus® is explained. Figure A.3 presents a scheme of the subroutine:

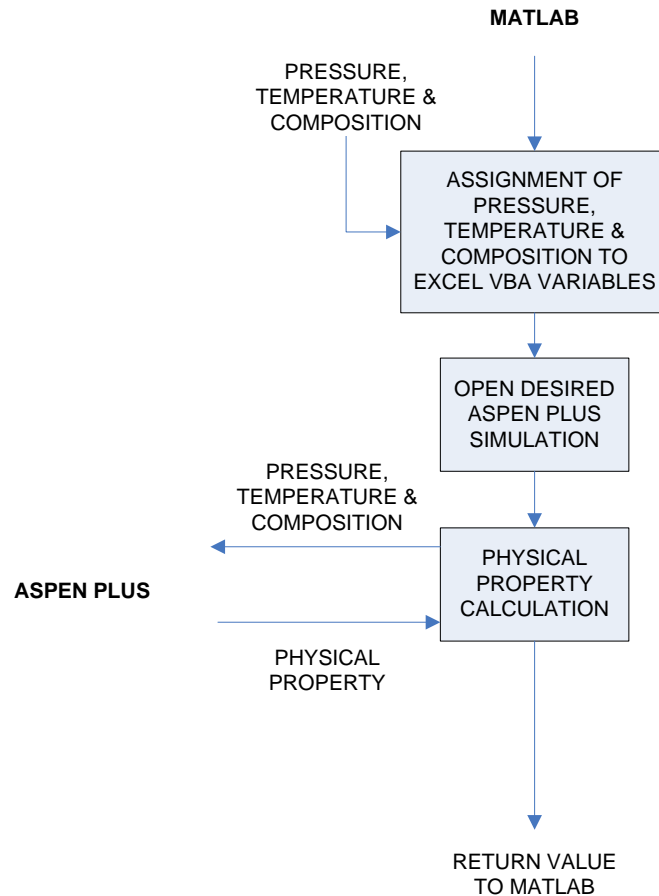


Fig. A.3. Scheme of the Excel VBA® subroutine which connects Matlab® with Aspen Plus®.

In the first step, the values of the pressure, temperature and composition which are received from Matlab® are stored in Excel® VBA variables. The Aspen Plus® simulation where the desired components and thermodynamic methods have been selected is initiated. The Excel® VBA subroutine transfers the values of the temperature, pressure and composition to Aspen Plus® and runs the simulation. Finally, the value of the physical property is read from Aspen Plus® and sent back to Matlab®.