Building novel equipment modules for a commercial process simulator: the compact plate heat exchanger case.

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Abstract

Process simulation is already a well-established method for process industry, useful to study the performance of either an individual unit operation or an entire plant. New types of equipment, which are in either an early stage of development or an experimental phase, are normally not included in commercial simulators, due to either lack of generalized design methods or limited interest in the specific piece of equipment, although their performance must be evaluated in conjunction with the available conventional equipment. *Aspen Custom Modeler* (*ACM*), which is a feature of the *Aspen Plus*® Engineering suite, is a convenient tool for non-experts for creating, editing, and re-using models of process units. Thus, the new equipment can be integrated with the conventional process equipment, in order to study its influence on the overall plant performance.

This work is a case study, where the plate heat exchanger design correlations are incorporated into an existing process simulator (*Aspen Plus*®). This type of heat exchanger was selected because it holds significant advantages over conventional equipment and is being rapidly adopted by food, chemical and refrigeration process industries. The paper gives an overview of the experience acquired in the course of the model integration procedure into the simulator.

1. Introduction

In recent years, industries are obliged to improve the performance of their plants and to reduce cost and time for plant development, in order to comply with economic, environmental and safety constraints. The use of a commercial process simulator has been proved a powerful tool both for the design and optimisation of chemical processes and for the evaluation of alternative designs. Its increasingly expanding application as an easy-to-use tool converts the computer into a virtual plant that can be used as a real alternative to the always expensive studies at pilot plant level.

Despite the fact that the commercial simulators offer a large number of advantages their use is limited to well-established unit operation models (e.g. distillation columns, conventional heat exchangers, reactors). Novel types of equipment, which are in either an early stage of development or an experimental phase, are normally not included in commercial simulators, due to either lack of generalized design methods or limited interest in the specific piece of equipment. However, there is need to incorporate novel equipment models in an existing simulator, in order to evaluate their performance in conjunction with the other plant equipment, since new research results slowly find their way into commercial process simulation software. To overcome this problem the majority of the existing simulators provide the possibility to import novel equipment models using additional software.

This work is a case study, where a novel piece of equipment, i.e. the compact heat exchanger, is incorporated into an existing process simulator (*Aspen Plus*®). In this way the new equipment can be integrated into the process and its influence on overall plant performance can be investigated. This paper depicts the experience obtained during the implementation of the new model into the simulator.

2. Integrating new equipment in a process simulator

In this study the *Aspen Plus*® is employed. It is a process simulator that uses the block-oriented approach, where, in order to study a particular unit operation, a set of design equations is implemented. Thus, each block, i.e. set of design equations, is a modelling component intended to perform a well-defined function, e.g. the simulation of a particular unit operation, or the numerical solution of certain types of optimization problems. This simple and effective approach helps engineers in solving standard flow sheets, but does not sufficiently support the solution of more complex problems. This is largely due to the multitude of models required in order to incorporate with sufficient details the numerous processing units encountered, such as multi-phase reactors, membrane processing units, polymeric reactors. On the other hand, some block-oriented process simulators, such as *Aspen Plus*®, give the possibility to introduce a novel piece of equipment and connect it to the conventional ones by simply importing in the simulator the equations that describe this particular type of equipment. Once the design equations plus the input and output parameters are defined, the new equipment can be integrated with conventional process equipment and its influence to the overall plant performance can be studied.

Several methods are provided for introducing new models in *Aspen Plus*® *11.1*. (Aspen Plus Manual, 2001) such as:

- **Fortran** subroutines, that can be implemented in the simulator in order to perform the calculations and extend the capabilities of *Aspen Plus*®,
- **Excel** spreadsheets that can be dynamically linked to the simulator in order to import or export process data
- Models that conform to the **CAPE-OPEN** (***C**omputer-**A**ided **P**rocess **E**ngineering*) standards, which were established with the goal of using process simulation tools de-

veloped by third parties within any standard chemical process simulation environment. These standards are based on universally recognized software technologies such as *COM* and *CORBA*, and are open, multiplatform, uniform and available free of charge (www.co-lan.org). *Aspen Plus*® provides support for part of the COM specification. (Aspen Plus Manual, 2001).

- **Aspen Custom Modeler** 11.1 (*ACM*), a special modelling language supplied by *Aspen Technology Inc*.

From the aforementioned methods, the one employed in this study, is the *ACM* which is a feature of the *Aspen Plus*® Engineering suite. *ACM* uses an object-oriented modelling language, editors for icons and tasks, and Microsoft Visual Basic for scripts to build simulation applications. In this way a block can be built, where the appropriate design equations are introduced and the input/output variables are defined and linked dynamically with other available process equipment (Aspen Plus Manual, 2001). Consequently, *ACM* can be considered a convenient tool for non-experts for incorporating new process units in the simulator, whereas *CAPE–OPEN* is more suitable for end-users with sound programming experience.

ACM can cope with different kinds of problems such as dynamic, steady state, parameter estimation and optimization simulations using an equation-based approach (Aspen Custom Modeler*TM* Manual, 2001). An important feature of *ACM* is that it provides direct access to the *Aspen Plus*® property database and in this way the physical and chemical properties of the various components involved can be calculated using the numerous property models offered by the simulator. In general the main steps that must be followed in order to implement a specific equipment model into *Aspen Plus*® using *ACM* are:

- The design equations that best describe the equipment behaviour must be chosen and the model input and output variables must be decided. The system of equations must have zero degrees of freedom.
- The components that are involved in the simulation model must be declared and saved in an *Aspen Properties file*, where also the most suitable property calculation method provided by *Aspen Plus*® is included. This file is used within *ACM*, where the components should be declared again.
- The variables involved in the equations are declared and assigned to the corresponding physical quantity and by default to its base unit.
- The design equations of the new unit operation model are inserted using *ACM* modelling language. Unlike conventional programming languages, *ACM* has no restrictions regarding the form and the solution order of the equations.
- The model *input* and output *streams* must be declared and assigned to an *input* or an *output port,* respectively. These ports are basically submodels which are added to the new model for dynamic information exchange with other *Aspen Plus*® blocks. All the variables of the *input port* are fixed and are assigned the values of the stream connected to the port, whereas the variables of the *output port* are free and are calculated during the simulation. In order to be able to incorporate the new model to *Aspen Plus*® the C^{++} compiler must be available.

The new equipment model, after being exported to the *Aspen Plus*® environment, can be connected to other equipment via the corresponding *input/output ports* and can be manipulated like any other block contained in *Aspen Plus*® library. It should be mentioned that the components must have ***identical*** names in the *Aspen Plus*® simulation, in the *Aspen Properties file* and in the *ACM* model.

3. Case study: The compact heat exchanger

In recent years, the requirement for energy-efficient heat transfer equipment is constantly increasing. In the same time the development of novel equipment has been driven by the need for economical, high performance, small in size and lightweight alternatives. The new generation of *compact heat exchangers* (*CHE*) complies with the above requirements. Compact plate heat exchangers comprised of surfaces with special modulations (corrugations) (***Figure 1***) hold significant advantages over conventional equipment, e.g. large surface area to volume ratio, enhanced heat transfer coefficients, ease of cleaning and inspection (Kays & London, 1998). Thus, they are commencing to widely replace conventional equipment, such as shell-and-tube heat exchangers, being rapidly adopted by food, chemical and refrigeration process industries. Moreover, due to the Greenhouse effect, the need for waste energy dissipation reduction becomes crucial. This kind of heat exchangers play an important role in the effort of preventing pollution caused by the emission of volatile organic compounds (e.g. VOCs, NOx), wastewater discharges (thermal pollution) etc.

Unfortunately, unlike the conventional heat exchangers, there is lack of a generalized design method for plate heat exchangers, a fact mainly attributed to the great variety of corrugation types and to the proprietary nature of the details of each particular design (Shah & Wanniarachchi, 1991). However, there are reliable correlations describing the performance of specific types of compact heat exchangers, like the chevron type (herringbone) compact heat exchanger, which is widely used in industrial applications.

Figure 1 shows a commercial compact heat exchanger comprising of adjacent corrugated plates, while the details of the plate are shown in ***Figure 2***. Each plate has herringbone type corrugations and two adjacent plates are superposed so that the opposite corrugations form a cross-type pattern with the crests of the corrugations nearly in contact. The corrugation type and angle affects the heat exchanger performance (i.e. the heat transfer rate and the pressure drop) (Shah & Wanniarachchi, 1991).

In addition, there is a number of possible flow arrangements (***Figure 3***) depending on the required heat transfer duty, available pressure drop, minimum and maximum allowable velocities and the flow rate ratio of the two fluid streams. Shah & Wanniarachchi (1991) classify them as series, looped and complex:

- The series flow arrangement (***Figure 3a***) is used for small flow rates and very close temperature approaches. Each flow passage corresponds to a pass. Thus the N pass-N pass arrangement consists of (2N-1) thermal plates. A pass in a *CHE* refers to a subsection of the exchanger (a group of channels) in which the whole fluid stream on one side flows one full length of the plate.
- Looped patterns are the most frequently used and are suitable for large flow rates, but relative small temperature differences on each fluid side. There are two types of looped patterns the *U*- (***Figure 1*** & ***3b***) and the *Z*- (***Figure 3c***) arrangement.
- The complex flow arrangement (***Figure 3d***) results by combining *Z*-arrangements in series, with generally identical number of thermal plates in each pass and are preferred when there is a significant difference in the flow rates of the two fluid streams and in the corresponding available pressure drops.

In the present work, the *Aspen Custom Modeler* (*ACM*) is applied, in order to introduce in the commercial simulator *Aspen Plus*® the module of a herringbone type plate heat exchanger. A typical *CHE* with looped flow arrangement was chosen as case study because this type is the most widely used. The design equations are identical for both *U*-and *Z*-type arrangement. However, if a series or a complex flow arrangement is to be studied the programmer must modify the correlations for the pressure drop prediction. The novel equipment modelled in *ACM* is used within *Aspen Plus*®.

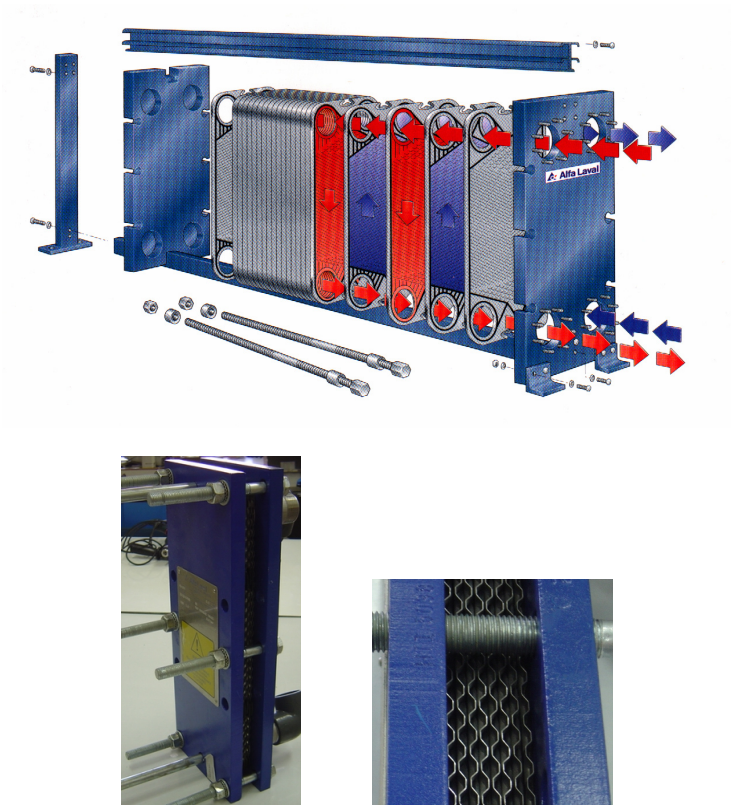

Figure 1. A typical plate heat exchanger (*by Alfa Laval*)

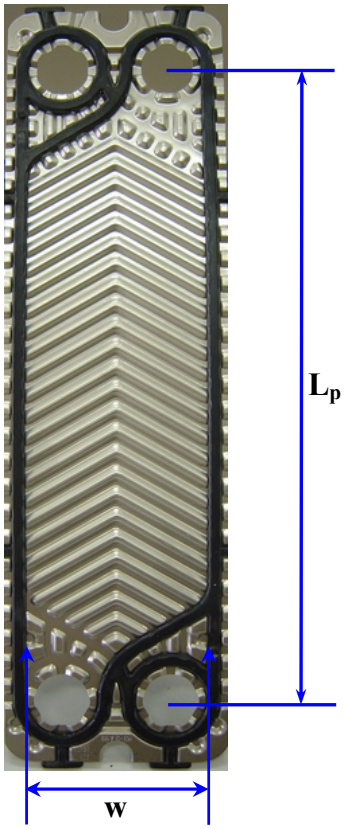

Figure 2. View of a corrugated plate

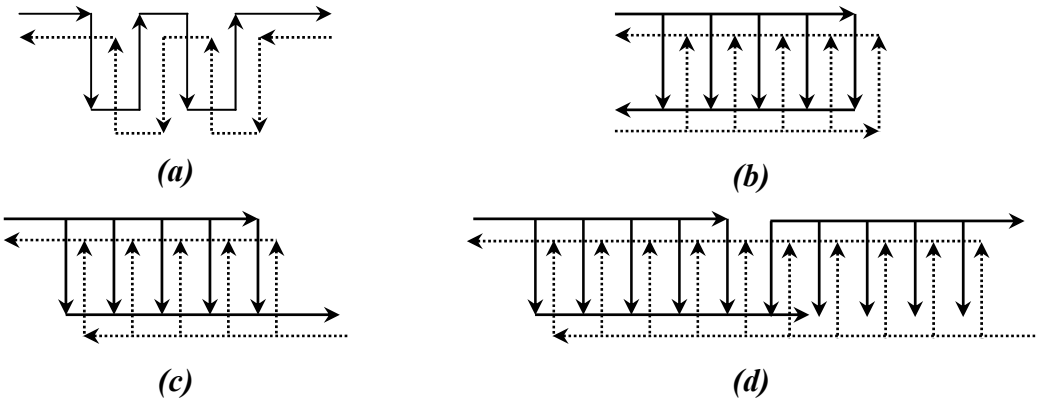

Figure 3. Basic flow patterns in a *CHE*: *(a)* Series arrangement or N pass-N pass with individual passes per channel, *(b)* Looped arrangement of *U*-type, *(c)* Looped arrangement of *Z*-type, *(d)* Complex arrangement (Shah & Wanniarachchi, 1991).

Design Equations

The model used in this study is the one proposed by Martin (1996) that predicts the friction factor and the heat transfer coefficient of a herringbone type *CHE* as a function of the corrugation inclination angle and the fluid Reynolds number. This model, which is based on a purely theoretical equation (i.e. a generalized Lévêque equation) as well as on experimental data, has been used by various investigators (e.g. Wang & Sundén, 2003). Moreover, Prabhakara Rao et al. (2002) consider this model the best available, although its predictions have ±20% uncertainty.

The model calculates the overall heat-transfer coefficient and the friction factor of a *CHE* as a function of its geometric characteristics (e.g. corrugation angle) and the fluid Reynolds number. The characteristic length used in the calculations is the hydraulic diameter, d_h, which is defined as:

$$d_h = \frac{4 \cdot \hat{a}}{\Phi} \tag{1}$$

The area enlargement factor, Φ, is the ratio of the developed surface area to the projected area and is defined as:

$$\Phi(x) \approx \frac{1}{6} \cdot \left(1 + \sqrt{1 + x^2} + 4 \cdot \sqrt{1 + \frac{x^2}{2}} \right) \tag{2}$$

where x is a dimensionless parameter defined as:

$$x = \frac{2 \cdot \pi \cdot \hat{a}}{\Lambda} \tag{3}$$

and depends on the ratio of amplitude $\hat{a}$ to the wavelength Λ. The geometric characteristics of a plate are shown in ***Figure 4.***

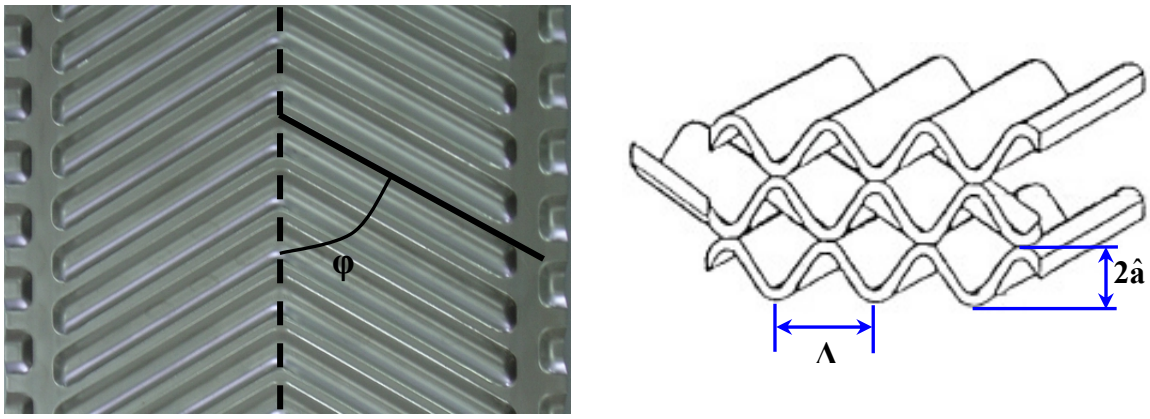

Figure 4. Geometric characteristics of a herringbone type plate.

The friction factor, ξ, is calculated by the equation:

$$\frac{1}{\sqrt{\xi}} = \frac{\cos(\varphi)}{\sqrt{b \cdot \tan(\varphi) + c \cdot \sin(\varphi) + \frac{\xi_o(Re)}{\cos(\varphi)}}} + \frac{1 - \cos(\varphi)}{\sqrt{\xi_1(Re)}} \tag{4}$$

Thus, the friction factor apart from the Reynolds number depends on the corrugation angle, φ. The friction factors at angle 0^o with the corrugations of the two plates shifted by π, so that the crests of the corrugations to be in contact, ξ_o, and at angle 90^o, ξ_1, are involved in the equation and are given by:

$$\xi_o = \frac{B_o}{Re},\ Re < 2000 \tag{5}$$

$$\xi_o = \left(1.81 \cdot g \cdot Re - 1.5\right)^{-2},\ Re \geq 2000 \tag{6}$$

$$\xi_1 = a \cdot \xi_{1o}\left(Re\right),\ a \geq 1 \tag{7}$$

The parameters *a, b* and *c* are predicted by fitting a curve to experimental data and are set to the values of 3.8, 0.18, 0.36 respectively, whereas the constant B_o can be predicted from ***Figure 5*** (White, 1991). Furthermore, the friction factor at angle 90^o and phase 0 (i.e. no contact points between the two plates), ξ_{1o}, is calculated by:

$$\xi_{1o} = \frac{B_1}{Re} + C_1,\ Re < 2000 \tag{8}$$

$$\xi_{1o} = \frac{K_1}{Re^n},\ Re \geq 2000 \tag{9}$$

The constants B_1, C_1 and K_1 depend on the area enlargement factor according to the equations:

$$B_1 = \frac{B_{1e}}{\Phi^2} \tag{10}$$

$$C_1 = \frac{C_{1e}}{\Phi} \tag{11}$$

$$K_1 = \frac{K_{1e}}{\Phi^{1+n}} \tag{12}$$

The values of the constants B_{1e}, C_{1e}, K_{1e} and n have been extracted from the experimental results of Focke et al. (1985) and have the following values: B_{1e}=1280, C_{1e}=5.63, K_{1e}=63.8 and n=0.289.

The Reynolds number, *Re,* is calculated using the superficial velocity, u, the viscosity, μ, and the density, ρ, of the fluid according to ***Eqs***. (13), (14), (15).

$$Re = \frac{\rho \cdot u \cdot d_h}{\mu} \tag{13}$$

$$u = \frac{\dot{Q}}{A_{flow}} \tag{14}$$

$$A_{flow} = 2 \cdot \hat{a} \cdot w \cdot n_{channels} \tag{15}$$

where $\dot{Q}$ is the total volumetric flow of each fluid of the *CHE*, A_{flow} is the average flow cross-section and $n_{channels}$ is the number of channels in which the flow is distributed.

The overall pressure drop, ΔP, for each fluid of the compact heat exchanger is given by:

$$\Delta P = \frac{\xi \cdot Re^2 \cdot L_p \cdot \mu^2}{2 \cdot d_h^3 \cdot \rho} \tag{16}$$

The dimensions of the plate (w, L_p) are defined in ***Figure*** 2.

It is considered that each fluid makes one pass inside the *CHE* and therefore the number of plates required for the heat exchange is calculated using ***Eqs.*** (17) to (20).

$$n_{plates} = \frac{A_{req}}{w \cdot L_p \cdot \Phi} \tag{17}$$

$$Q = \dot{m} \cdot c_p \cdot \left| T_{in} - T_{out} \right| \tag{18}$$

$$Q = A_{req} \cdot U \cdot \Delta T_{ln} \tag{19}$$

$$\Delta T_{ln} = LMTD = \frac{\left(T_{hot_{in}} - T_{cold_{out}} \right) - \left(T_{hot_{out}} - T_{cold_{in}} \right)}{\ln\left(T_{hot_{in}} - T_{cold_{out}} \right) - \ln\left(T_{hot_{out}} - T_{cold_{in}} \right)} \tag{20}$$

where the required area for heat transfer, A_{req}, is calculated from the fraction of the total heat exchanged, Q, to the overall heat transfer coefficient, U, and to the mean logarithmic temperature difference, ΔT_{ln}. Also, the total heat transferred is proportional to the mass flow rate of the fluid, $\dot{m}$, the specific heat capacity, c_p, and the input, T_{in}, and output, T_{out}, temperature of one of the fluids used in the *CHE*. It should be mentioned that for operational reasons a *CHE* must be comprised of an odd number of plates, so as the *CHE* to include an equal number channels for the hot and the cold fluid.

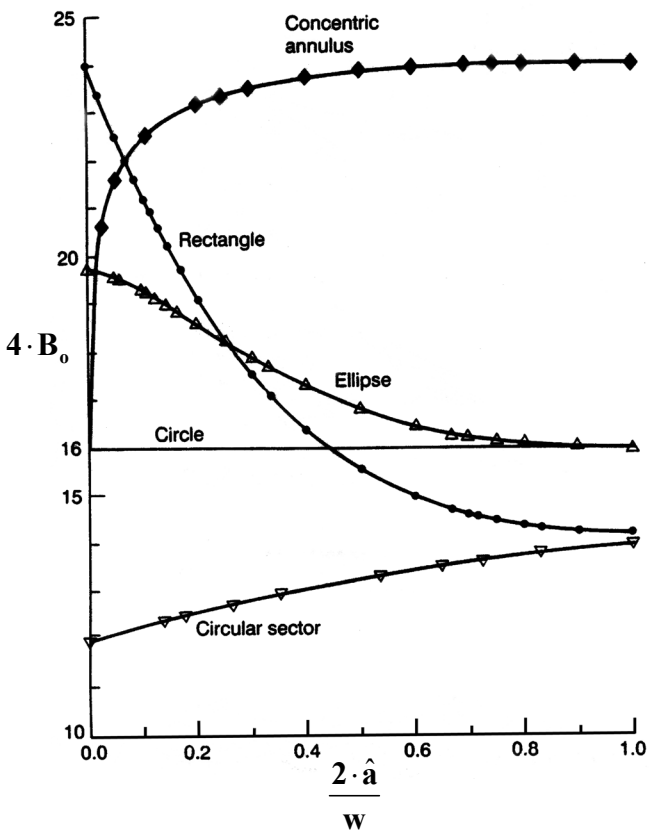

Figure 5. Values of constant B_o vs duct cross section (White, 1991).

In addition to the pressure drop, the overall clean heat transfer coefficient, U_c, is calculated using the cold and hot side partial heat transfer coefficients, h_{cold} and h_{hot}:

$$\frac{1}{U_{clean}} = \frac{1}{h_{hot}} + \frac{\Delta x}{k_{ss}} + \frac{1}{h_{cold}} \tag{21}$$

In ***Eq.*** (21) the ratio of the plate thickness to the plate thermal conductivity, $\frac{\Delta x}{k_{ss}}$, is considered to have a higher value than the other two and therefore it is neglected.

Both partial heat transfer coefficients are calculated using the Nusselt, *Nu,* and the Prandtl, *Pr,* number as shown in the following correlations:

$$Nu = 0.122 \cdot Pr^{1/3} \cdot \left(\frac{\mu}{\mu_w}\right)^{1/6} \cdot \left[\xi \cdot Re^2 \cdot \sin\left(2 \cdot \varphi\right)\right]^{0.374} \tag{22}$$

$$Nu = \frac{h \cdot d_h}{k} \tag{23}$$

$$Pr = \frac{\mu \cdot c_p}{k} \tag{24}$$

where *k* is the thermal conductivity of each fluid. In addition, the property ratio correction, i.e. the ratio of the viscosity at the average temperature of each side to the viscosity at the wall temperature, $\left(\mu / \mu_w\right)$, in practice is taken equal to one (Kern, 1965). Finally, the overall heat exchange coefficient is calculated from the clean overall heat transfer coefficient and the dirt factor, R_d, as follows:

$$\frac{1}{U} = \frac{1}{U_{clean}} + R_d \tag{25}$$

The physical properties used in the above correlations are calculated at the average temperature, T_{av}:

$$T_{av} = \frac{T_{in} + T_{out}}{2} \tag{26}$$

It is obvious that all the aforementioned equations are used for calculating the overall heat transfer coefficient and the pressure drop of both cold and hot fluid. In case that the flow pattern is changed the correlations for the pressure drop calculations must be modified accordingly. It is noted that all the variables must be expressed in SI units.

Programming procedure

The independent (fixed) and dependent (free) variables of the model are defined (***Table 1***) so as the degrees of freedom are zero. After declaring the components of the new model in both the *Aspen Properties* and *ACM* files the following steps are carried out:

- All variables are declared and assigned to their corresponding physical quantity and to its SI base unit. The variable status is also assigned (***Table 1***) but it can be changed afterwards by the user.
- The model input and output streams are defined i.e. the input and output streams for both sides of the *CHE*.
- Four submodels are built for the calculation of all physical properties required, which can be called from within the main program whenever it is needed. The four submod-

els correspond to the cold and hot fluid and the two possible fluid conditions (i.e. gas or liquid).

- The design equations of the *CHE* (***Eqs.1-26***), as well as the mass and energy balances, are written using *ACM* format.
- The model is compiled with *ACM* compiler and run in steady state mode.
- The *input* and *output* ports are assigned to the input and output streams. The ports used are the default SI-ports provided by *ACM*. The model is run again in steady state mode.
- Finally, it is compiled using the C^{++} compiler and the resulting *dll* file is exported to the same folder with *Aspen Properties* file.

In order to use the new model in an *Aspen Plus*® simulation the module must be introduced from the Library (in the *References* menu) and it appears in the *Model Library* bar. From this point the new module can be manipulated from within the simulator environment.

Table 1. Variables of a *CHE*

	Variables
Physical properties	c_p, k, k_{ss}, μ, μ_w, ρ
Fixed (input) variables	a, $\hat{a}$, b, B_{1e}, c, C_{1e}, K_{1e}, L_p, $\dot{m}$, n, $\dot{Q}$, R_d, T_{coldin}, T_{hotin}, w, ΔT_{hot}, Δx, Λ, φ
Free (calculated) variables	A_{flow}, A_{req}, B_1, C_1, d_h, h_{hot}, h_{cold}, K_1, $n_{channels}$, n_{plates}, Nu, Pr, Q, Re, T_{av}, u, U_{clean}, U, x, Δp, ΔT_{cold}, ΔT_{ln}, ξ, ξ_1, ξ_o, ξ_{1o}, Φ

The modelled *CHE* was introduced in *Aspen Plus*® and was validated using the data of Martin (1996). Furthermore, the new equipment was integrated with conventional process equipment and it was found to function very well.

4. Conclusions

With the intention of reducing cost and time for plant design and optimization, process simulation has become a vital tool. However, the equipment library offered by commercial process simulators is usually limited to conventional equipment and must be enhanced by new equipment, the performance of which need to be studied in conjunction with conventional ones.

ACM is a modelling language provided by *Aspen Plus*® that is intended for users with minimum programming skills. The user is allowed to introduce all the required model equations in the form that they are available in the literature, i.e. without having to bring them in a y=f(x) form. Additionally, the equations can be arranged regardless of the order that they are going to be solved. The new model can be easily incorporated in the process simulator and has full access to the build-in routines for the physical properties estimation. Moreover, the input and output variables can be easily interchanged (i.e. without altering the computer code) from within the main simulation.

However, there are several drawbacks in using an exported *ACM* model. For example, the components, the parameters and the physical property method used in the novel equipment can be altered only within *ACM* environment. Additionally, the component names must be explicitly declared and identical names must be used in the *ACM* model, in the *Aspen Properties file* and in the *Aspen Plus*® simulation run. Sensitivity analysis, which is a

powerful tool that helps design engineer to locate the crucial parameters, whose variation greatly affects the overall plant performance, can not be conducted using the model variables either as manipulated (i.e. input) or calculated (i.e. output) variables. However, the model can be included in a sensitivity analysis run which concerns the other process variables.

Finally, it is up to the user of this programming tool to decide whether the simplicity of the *ACM* tool compensates its limitations.

6. References

1. Aspen Custom Modeler™ Manual 11.1, 2001. AspenTech.
2. Aspen Plus 11.1 Manual, 2001. AspenTech.
3. Focke W.W., Zachariades J., Olivier I., 1985. The effect of the corrugation inclination angle on the thermohydraulic performance of plate heat exchangers, *Int. J. Heat Mass Tranfer*, **28**(8), 1469-1479.
4. Martin H., 1996. A theoretical approach to predict the performance of chevron-type plate heat exchangers, *Chemical Engineering and Processing*, **35**, 301-310.
5. Kays W. M., London A. L., 1998. Compact Heat Exchangers, 3rd Edition, Krieger Publishing Company.
6. Kern D.Q., 1965. Process Heat Transfer, McGraw-Hill.
7. Prabhakara Rao B., Krishna Kumar P., Sarit Das K., 2002. Effect of flow distribution to the channels on the thermal performance of a plate heat exchanger, *Chemical Engineering and Processing*, **41**, 49-58.
8. Shah R.K., Wanniarachchi A. S., 1991. Plate heat exchanger design theory, In: Buchlin J-M. (Ed.), *Industrial Heat Exchangers*, von Karman Institute Lecture Series 1991-04.
9. Wang L., Sundén B., 2003. Optimal design of plate heat exchangers with and without pressure drop specifications, *Applied Thermal Engineering*, **23**, 295-311.
10. White F. M., 1991. Viscous Fluid Flow, 2nd Edition, McGraw-Hill International Editions.