First-principle simulation for thermo-hydraulic engineering

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Abstract. AHTL (A Heat Transfer Language) is a tool for thermo-hydraulic simulations, based on first principles. AHTL is currently under development. Its purpose is to modernize existing engineering tools. This paper outlines how traditional engineering methods, Object-Oriented software design and numerical methods can be combined to provide functionality not found in existing equipment design software. AHTL provides first principle models for fluid balances, conduction and heat transfer. The related equations are solved by a direct solver. Virtually any heat exchanger can be modeled. A discerning feature is the strong data-orientation of the models used. Data-orientation facilitates interfacing to databases and integrating design cycles and company work processes. This paper mainly focuses on the principal ideas and the practical implications. As AHTL is developed into a commercial product, more results will become available.

1 Traditional methods

Heat transfer engineering has a longstanding history. Traditional heat transfer equipment design software is usable and does yield trustworthy results. Examples of this software are design and rating programs for shell and tube exchangers, plate exchangers, aircoolers, and fired heaters.

Traditional heat transfer equipment design software is based on methods that were developed before 1950 [2,3,4]. These methods go to great lengths to minimize the burden of manual calculation. Depending on the equipment type, specific physical phenomena are neglected (e.g. radiation, static pressure differences). This may cause incorrect results for extreme operating conditions. The use of simplifying assumptions puts the burden on the engineer to check their validity. This procedure is cumbersome and error-prone, especially when large complex installations are analyzed for a large number of operating conditions. Furthermore, the organisation of engineering data and calculations in current software applications appears to be outdated, which sometimes makes it difficult to use. Traditional software often contains limitations, such as the maximum number of equipment components, which are unnecessary nowadays. This makes it inflexible. It can force the engineer to split up his simulations or even make calculation impossible.
The methods contain implicit knowledge of the lay-out of a specific type of heat transfer equipment. The computer applications implement these methods directly and mix up numerical solution with engineering calculations. They lack a consistent philosophy on data structures and they combine the above aspects in a non-systematic manner. This may lead to inefficient nested iterations and even instabilities such as limit cycles. Traditional software can only calculate steady state. Transients, such as start-up, shut-down or emergencies, can not be analyzed.

The traditional approach requires a dedicated computer program for each type of heat transfer equipment. All these different programs together result in high licence and software maintenance costs. Traditional design programs are not designed to exchange data between each other. Determining the total response of a flowsheet containing different types of equipment adds interfaces between the dedicated calculation tools and another level of iterations. Numerical convergence can be problematic. Furthermore, the cost of interfacing dissimilar software tools is high. Traditional computer applications are not designed to exchange data with other design or business applications. The lack of integration between engineering tools within a design department but also between different departments causes high costs because of tedious manual re-input, checking and undetected errors. The fact that a number of these traditional design tools generate equipment data sheets and have been integrated with process simulators to obtain fluid property data does not overcome many fundamental drawbacks of their basic design. Furthermore, links between software components are often proprietary.

In conclusion, neglecting specific physical phenomena or using special shortcut calculation methods to reduce manual calculation effort has numerous drawbacks. Modern computers do not require one to simplify the models and the simultaneous solution of a set of difference equations is even remarkably efficient compared to the many nested iterations found in traditional applications. Important gains in design quality and in the reduction of engineering costs can be achieved by looking for common ground instead of looking for special properties.

2 Conservation laws

Today, there is a growing tendency to make use of similarities (laws of physics) instead of exploiting specific equipment properties. Eventually, the laws of physics are equally valid for all heat exchangers. Many advanced tools that support this approach are nowadays available [6-10]. Despite this, tools that are based on first principles are not yet routinely used in everyday engineering. Traditional tools are generally used for "rigorous" equipment design calculations. Although the heat transfer and pressure drop correlations used are based on expert know-how, the software design concept of many of these packages appears to be outdated. This can burden the user with unnecessary work as outlined in section 1 above. A fundamental approach is not an end in itself. In the past, such methods have only been applied for demanding applications such as nuclear engineering or space travel. This approach should no longer be considered cutting-edge technology. NASA started to perform comparable calculations in the 1960's [5]. AHTL uses finite difference methods, as opposed to Computational Fluid Dynamics. For day-to-day engineering and design problems, finite difference methods are sufficiently accurate and they are flexibile in describing the equipment and in providing data exchange capabilities.

AHTL should not be compared to advanced equation-based simulators. These offer full flexibility, but programming and using them requires expert knowledge. Writing a heat transfer simulator comparable to ATHL in equation based form is a major undertaking and as of today, the author is not aware of such design tools. AHTL is positioned between the traditional tools and equation-based simulators. Conservation laws are implemented in an object-oriented manner, and the result is flexible and powerful.

3 Main Models

The back-bone of AHTL is formed by a small number of first principle physical models, which have been hard-coded. The result is very versatile. The two most important models are the heat conduction in solids and the fluid balances, described in section 3.1. Model data structures are special in that they form a fully closed decomposition system of the thermo-hydraulic problem data structure. This is a very important feature, as it significanly facilitates equipment modeling. The first principle submodels provide each other with the relevant physical data just by reference, hiding all internal complexity. This is a typical property of Object-Oriented software design [1]. The Object-Oriented design also leads to a high degree of re-using models. No other heat transfer equipment engineering software tools are known today with this property. Classical heat transfer and pressure drop engineering correlations can be employed within AHTL, but so can more advanced models. The main models are described below.

3.1 Fluid balances

The fluid balances are one-dimensional, so that the fluid thermodynamic state varies along the length of the stream only. The stream model contains four submodels: fluid property model, mass balance, impulse balance and energy balance.

3.1.1 Fluid Properties

A straightforward model for fluid properties is implemented. This model utilizes tabulated values for single and mixed phase. The fluid properties are determined using linear interpolation within the property table. If the thermodynamic state is outside the table, this error is flagged. Mixed phase is modeled as homogeneous phase. Fluid property tables can be defined at various pressure levels. There is neither a limit to the number of pressure levels nor to the number of temperature data points, at which fluid properties are given. On the other hand, the fluid property interpolation routines can also handle a minimal set of data points, as long as it makes sense. Fluid property calculation is always external.

3.1.2 Mass Balance

The mass balance is posed as an algebraic equation, meaning that there is no varying mass storage in a fluid control volume. As a consequence, it is not possible to calculate shock waves or water hammer in piping. These processes play on a split second time constant base. They are not useful for the normal thermo-hydraulic problem but would reduce the integration time step size considerably.

3.1.3 Impulse Balance

The impulse balance is fully implemented, including static heads and acceleration losses due to flow area changes. It is also solved algebraically. It is not possible to assess time dependent acceleration, such as establishing a flow velocity in a previously stagnant stream due to opening of a valve. In practice, however, the valve opening process is in most cases slower than the time it would take to accelerate the stagnant fluid column. Friction pressure drop models can be specified along the lines of the traditional correlations. Friction pressure drop is calculated as a resistance factor times the velocity head. The resistance factor ζ can be specified using:

$$\boldsymbol{\zeta = A + B * Re^{C}} \qquad [1]$$

In case this is not deemed adequate, a built-in interpreter can execute user/template (see sec.5) supplied statements.

3.1.4 Energy Balance

The energy balance fully implements the first law of thermodynamics. The energy balance model is solved dynamically in the time domain. The primary quantities describing the fluid state are velocity, static pressure and enthalpy. It is possible to specify the enthalpy that includes the heat of reaction. Chemical reactions can then be handled just by mixing fluids. Reaction models are external as is all fluid property calculation.

3.2 Heat Conduction in Solids

The heat conduction model is also one-dimensional. It is thus assumed that the heat flow is always perpendicular to a wall. The model is implemented for flat, cylindrical and spherical walls.

3.2.1 Solid Properties

The simulation automatically takes solid property variations into account. While this is not of great importance for heat exchanging areas such as tube walls, which have a low thermal resistance, it is especially useful for heat insulating materials whose conductivities often exhibit a significant dependence on temperature. The specific heat and the thermal conductivity are tabulated for solid materials and the program uses linear interpolation between the values provided.

3.2.2 Capacitance-Resistance model

A solid wall is modeled according to the well-known capacitance-resistance model and it can be composed of one or more layers. Each layer can consist of a different construction material. Thermal nodes are placed at each layer interface. As a minimum, a wall consists of one layer, which gives rise to two capacitance nodes and one resistance node. A wall always has two surfaces.

3.3 Heat Transfer

Heat transfer models couple the fluid balances and solid conduction models. Wall and stream spatial discretisation, together with the connection geometry specify a heat exchanger. One convective and three radiant ones (solid-solid, gas-solid, gas-gas) heat transfer models are foreseen. Many engineering type convective heat transfer coefficients can be described by the correlation

$$U = (1-x) \{ a_l + b_l * Re_l^{c_l} * Pr_l^{d_l} * (\mu_b/\mu_f)^{e_l} \} + x \{ a_v + b_v * Re_v^{c_v} * Pr_v^{d_v} * (T_b/T_f)^{e_v} \} \qquad [2]$$

Where this approach is considered inadequate, arbitrary heat transfer correlations can be calculated using a built-in interpreter executing user or template-supplied (see sec.5) statements.

Logarithmic Mean Temperature Differences (LMTD's) are approximated by a number of direct temperature differences. Already a small number of direct temperature differences approximates the LMTD well (2% with 5 direct differences, 0.5% with 10). However, the LMTD itself assumes that the specific heat is constant for both process sides. This is hardly ever true for any sizeable temperature range, let alone when vapourization is involved. Therefore, direct temperature differences will often be more accurate. This is all the more true as local heat transfer coefficients can be used instead of mean values. A radiant heat transfer model will be implemented. The model data structures are already implemented. The determination of radiant exchange factors will be included in the program.

4 Physical Abstraction layer

Basically, fluid streams and solid walls are independent entities. They are connected by heat transfer. A stream node can be bounded by an unlimited number of different areas. Streams can be split and combined. This allows modeling of arbitrary thermal networks. The above models, complemented with I/O routines and an interpreter for general calculations (also for process control), form a physical abstraction layer that allows generic modeling of heat transfer equipment. Notably, any physical quantity within the simulation is accessible to the interpreter or can be modified by it. Any quantity can be output using generic I/O routines.

This has the following properties:

1. The fundamental models are implemented in an Object-Oriented fashion. All relevant physical quantities are taken into account and attributed to the proper submodels. In this way, each and every datum pertinent to the heat transfer process, without omission or repetition, is stored within the submodels. A small number of model types is sufficient to model virtually any type of heat exchanger. Model building is much simplified using these fundamental objects. Objects just have to refer to each other to obtain the relevant physical data from the other objects.
2. Any engineering method can be applied, because all relevant data is available. Any type of heat exchanger can be modeled in virtually any detail desired. By choosing traditional correlations for friction pressure drop and heat transfer, as well as the spatial discretisation to suit, any equipment type can be modeled in a manner that -in principle- gives identical results compared with the original traditional program, but without its drawbacks.
3. Numerical solution is internal to the fundamental models. The model builder can forget about it. A sparse direct solver solves a set of semi-implicit differential equations.
4. Transient as well as steady state simulations can be done. Transient responses are helpful in assessing start-up and shut-down as well as emergency situations and control strategies.
5. The fact that the modeling basis is identical for all types of heat transfer equipment, makes flowsheet calculations containing different types of heat exchangers easy. The models of the various heat exchangers speak each other's language and no conversion or interface is necessary between them at all. Complex stream networks can just be built from the low level physical models available.

5 Template Applications

A heat exchanger is modeled by a small number of fundamental physical models, but using a large number of nodes. Providing the input for these manually is possible but not practical for a design engineer. Therefore, for each type of equipment, a template application should be provided. This template generates the low level model input from customary engineering data and specific knowledge about the equipment (such as correlations and geometric design data) that is built into the template application. In this way, the thermal engineer can use AHTL in roughly the same manner as familiar equipment design applications. AHTL is targeted at thermo-hydraulic engineering of process heat transfer equipment such as shell and tube, plate exchangers, ducting, heat recovery systems, but it is not limited to these.

6 Numerical solution

The models for heat conduction and those for the fluid balances, both including all their submodels, have been implemented and tested independently. To illustrate the kind of results that AHTL can produce, two examples are given in figures 1a and 1b. Test cases have been either taken from literature or were validated by other means. All dynamic models are integrated using a semi-implicit integration method. The heat conduction problem yields a tridiagonal matrix that can be efficiently solved using the Thomas algorithm. Boundary conditions for the heat conduction problem are the relevant process temperatures, heat transfer coefficients and surface areas. These were kept constant for the above tests, see figure 1a (at left) for an example. This example is a recalculation of a problem given in [11], which represents the convective heating of a resin slab that is divided into four layers (five nodes). The solid line is the exact solution. The solution with an overshoot comes from [11] where an explicit method is used. The solution that slightly lags the exact solution, which is as expected for a semi-implicit solution, is that from AHTL. The fluid balance equations lead to a matrix system with a diagonal and a subdiagonal that can be solved using direct forward substitution. The boundary conditions for a stream are the wall temperatures, areas and heat transfer coefficients. These were also kept constant for the tests, see figure 1b (at right). This figure shows the dynamic response of the development of the vaporization fraction in a hydrocarbon process flow. Initially, the enthalpy of all twenty-two fluid nodes is at inlet conditions. The graph shows the time response. The numerical integration is equipped with a method to automatically adapt the time step as a function of the integration error. The numerical behaviour and stability is excellent and systems containing time constants that are fractions of a second can be integrated using time steps in the order of a minute. The simulation results have been compared to results from other sources for the same problem and excellent agreement has been achieved. Other test cases can be seen on the website of Heat Transfer Consult, http://www.heattransferconsult.nl.

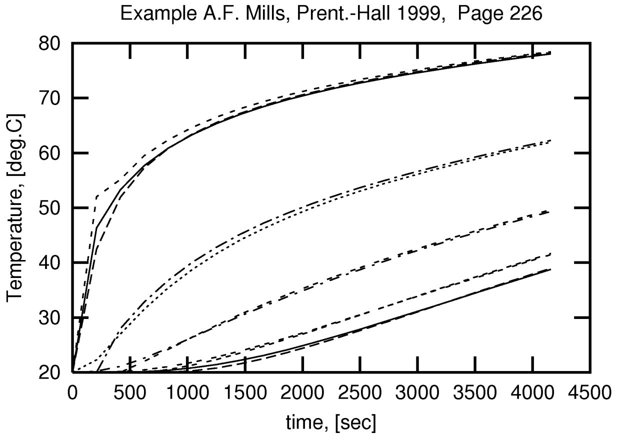

figure 1a

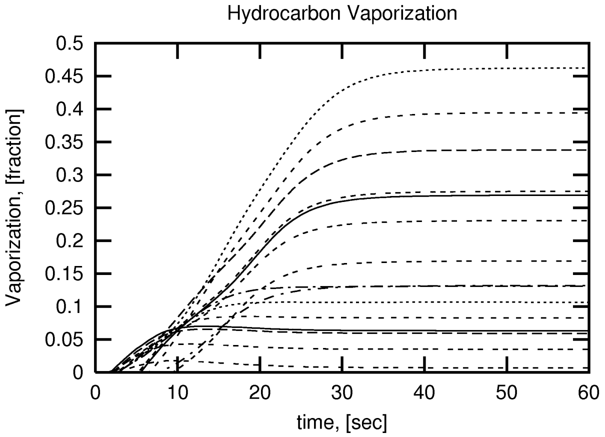

figure 1b

The next step is to combine the above two models (walls and streams) by coupling them via heat transfer. The connections made by the heat transfer process replace the static boundary conditions mentioned above. To preserve the stability of the semi-implicit integration scheme, it is necessary to solve the complete set of equations as a whole. The resulting square matrix contains some tens of equations for trivial problems, some hundreds for typical equipment engineering problems and some thousands for flowsheet calculations. The resulting matrix is large and sparse. The implementation of the sparse solver is currently in progress. Preliminary testing of the solver indicates that the ratio of simulated time over actual time for a system with 2500 equations and using an integration time step of 30 seconds will be at least 60 on a 600MHz i686 PC. As soon as the solver is implemented, more examples from literature will be recalculated and the results compared.

7 Conclusions

A small number of data structures is involved in the fundamental models. The universal decomposition of the heat transfer problem is an important feature. All physical data of any heat exchanger are projected onto this universal data structure. The Object-Oriented program structure greatly simplifies the modeling process. The only equipment-specific input are the correlations for friction pressure drop and heat transfer. Equipment is further specified by geometric connections within the thermal network, and straightforward data such as areas, volumes, locations and orientations. Template applications for detailed models are easy to write.

AHTL is intended to remove many drawbacks found in equipment rating programs that are used by engineering companies today. Specifically, it:

1. does away with the unnecessary limitations concerning the equipment geometry, size or type.
2. fully implements impulse and energy balances and thus yields valid results also in extreme operating conditions. It can handle fluid velocities up to sonic velocity.
3. can use traditional design correlations and -in principle- produces identical results compared with traditional design rating programs. In general, the answers will be more accurate because AHTL predominantly uses local quantities as opposed to mean values in traditional methods. Deviating results may also stem from item 2).
4. allows additional model sophistication and refinement.
5. can help the engineer by including aspects of the design process that were previously performed separately by hand (e.g. heat loss calculations).
6. can perform transient simulations.
7. projects all simulation data onto the same, universal, standardized data format. This data can subsequently be stored in databases, which facilitate integration of engineering competences and company work processes. This integration uses only open standards such as SQL and/or STEP-related protocols. This integration can be implemented by third parties.
8. applies templates to shield advanced features from the engineer, who does not need specific simulation expertise.

Important savings may be achieved by introducing better design tools. All the above properties of AHTL contribute to shorten design cycle time and to improve the quality of equipment design.

Nomenclature

A,B,C = Constants
Re = Reynolds Number
ζ = friction factor
U = Heat Transfer Coefficient [W/m^2/K]
x = vapour fraction
Re_l, Pr_l = liquid Reynolds and Prandtl numbers
a_l, b_l ,c_l ,d_l ,e_l = liquid heat transfer correlation parameters
Re_v, Pr_v = vapour Reynolds and Prandtl numbers
a_v, b_v ,c_v ,d_v ,e_v = vapour heat transfer correlation parameters
μ_b, μ_f, T_b, T_f = bulk and film viscosity and temperature

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