An integrated knowledge approach for conceptual equipment design

Ioa S. Gavrila
Artificial Intelligence Group
Department of Computer Science
Vrije Universiteit Amsterdam
e-mail: **ioa@cs.vu.nl**

Piet Iedema
Process Dynamics and Integration Group
Department of Chemical Engineering
University of Amsterdam

Abstract: This paper addresses two real life engineering design problems. A main design problem is the synthesis task: given a requirements specification and an unsatisfactory design, how should this design be changed in order to fullfil the specification ? When a satisfactory design has been found, it is often the case that only the values that describe this design are stored. Because all information about the origin of these values is lost, reuse of (parts of) the design is difficult and the same design problem is solved many times.

In this paper we describe a design system for heat exchanger design that automates and gives support for the main design tasks: synthesis, analysis and evaluation. Heuristic synthesis rules, qualitative and quantitative models have been integrated for use in the synthesis and analysis tasks. Causal graphs are used to justify the origin of variable values.

The system is equipped with explanation and advisory facilities. The design modifications proposed by the heuristic rules can be questioned, and in certain cases these rules are justified by the numerical models. Further, the system uses the qualitative model to help the designer in finding its own modifications. Finally, explanation facilities are present to trace the origin of design values, if necessary back through several design alternatives.

1. Introduction

A common engineering practice during the design process is the following. Given a requirements specification, the designer first decides on the design class to which the solution design will belong. The chosen design class is used to determine the mathematical model, that describes the variables of the system and their numeric relations. Then the input or exogenous variables are determined and promising values for them are chosen. Now the model can be solved: the values of all dependent variables are calculated. Finally the design is evaluated against the requirements, and if the design is not satisfactory a new design cycle is initiated.

In the case of conceptual equipment design for the process industry, the design classes describe the different types of equipment (e.g. a distillation column, an absorption unit). The system variables describe the geometry of the equipment (the design variables) and relevant properties of the incoming and leaving streams (the stream variables). The input stream variables together with a part of the design variables are used as the exogenous variables. From this information, the dependent design variables and the output stream variables are calculated. If the latter do not comply with the requirements, the geometry of the equipment must be changed (the input stream variables are fixed).

But how should the geometry be modified ? More concrete, which design variables to choose as exogenous variables and which values to assign to them ? It is not an easy task to make these decisions, because changing one aspect of the geometry can have favourable effects on some performance aspects but at the same time unfavourable effects on others. To solve this problem, we propose an integration of heuristic modification rules, qualitative models and mathematical models: the qualitative model is deduced from the mathematical model, and part of the heuristic rules are deduced from the qualitative model.

During the design process many design alternatives are developed until a satisfactory design is found. Once found, the values of the design variables are stored, but their justification is lost. Was this design decision adopted from the previous design or was it the result of other decisions ? Which model was used to calculate the pressure drop ? This kind of information is necessary to understand later on the design decisions, and to make reuse of (parts of) the design possible.

The outline of the paper is as follows. First an introduction is given in the chosen application domain: the design of heat exchangers. This domain has been analysed using the KADS methodology, and in section 3 the main parts of the conceptual model are presented: the design tasks, the knowledge types used (i.e. heuristic rules, qualitative and mathematical models) and their integration, and finally the type of information generated during a design cycle.

The KADS model has been used as starting point for the architecture of a design system. In section 4 we describe a design system that performs the main tasks identified in the conceptual model, and that has several explanation and advisory facilities. The paper concludes with a comparation with related work.

2. Design of heat exchangers

In many places in a chemical process, heat must be removed or added to the process streams. A common practice is to exchange heat between two streams. Expressed thermodynamically: heat from the hotter stream is used to increase the enthalpy of the colder stream. During this heat transfer a phase change might occur in one of the two streams (i.e. if the hot stream is in the vapour phase it may condensate, if the cold stream is in the liquid phase, it may evaporate).

Heat exchangers are designed for this purpose. There are many types of heat exchanger, and their suitability is determined by the situation, e.g. occurance of a phase change, the fouling (dirt) factors of the streams, the operating pressure of the heat exchanger (see [Yang e.a., 1993] for an expert system for heat exchanger selection). Of all types, the shell and tube heat exchanger is the most commonly used in chemical industries. We will restrict our discussion to this class of heat exchanger designs.

A typical shell and tube has the form of a cylindrical shell, in which three departments can be found (see figure 1) [Coulson e.a., 1983]. In the middle department the actual heat transfer takes place; it consists of a number of parallel tubes, fixed at their ends in tube sheets and supported in between by baffles. The tube sheets form the boundary between the middle department and the two outer departments, the heads.

One of the two fluids flows through the tubes, the *tube-side fluid*, the other around the tubes, the *shell-side fluid*. The tube-side fluid enters and leaves the shell and tube in a head. Often, this fluid is directed to flow several times back and forth through the tube bundle, to increase the heat transfer. To achieve these tube passes, the heads are partitioned with partition plates.

Also on the shell-side provisions can be taken to increase the heat transfer rate. First, the presence of baffles increases the fluid path because the shell-side fluid must now flow up and down through the shell. Second, also the shell-fluid can be directed to flow in more shell-passes.

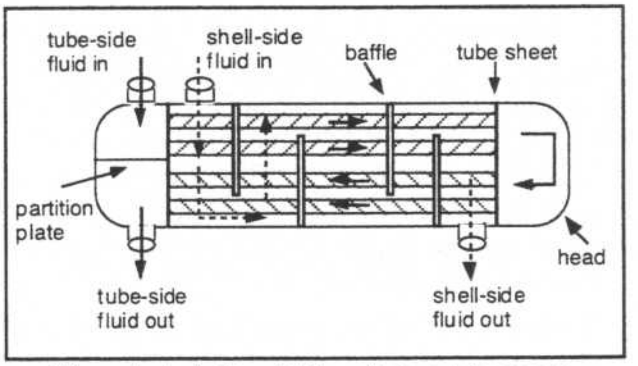

Figure 1. A shell and tube with two tube passes and one shell pass

Requirements specification and design procedure

A requirements specification for the design of a shell and tube typically consists of the following information about the two streams: the composition, the input and/or output temperature, the flow rate (kg/h) and the maximum allowable pressure drops. (Note that these variables are dependent on each other).

This information is used in the first place to determine the required duty of the heat exchanger, Q, and then to estimate the needed heat-exchange area, A. Once a heat exchanger has been designed, the actual area is known, and the actual duty can be calculated.

The following formula, that is the general equation for heat transfer across a surface, is used in both cases:

$$Q = U * A * \Delta T_m$$

where

Q = heat tranfer per unit time, Watt

U = overall heat transfer coefficient, Watt/m^2 °C

A = heat-transfer area, m^3

ΔT_m = mean temperature difference, °C

The U-term is the reciprocal of the overall resistance to heat transfer between the cold and hot fluid. It is the sum of several resistances:, the fluid film resistances of both fluids, the resistance of the tube wall, and the resistance caused by the dirt deposited on both sides of the tube wall.

When the required duty is calculated, the requirements information is used to calculate Q and ΔT_m. Because we don't have a design yet, the value of U must be estimated; now the formula is used to calculate the required area, A. Once there is a design, the actual values of A and U are known (calculated by other formula's) and now the formula is used to calculate Q. This illustrates that the same formula is used for different purposes, and that the same variable can be calculated in different ways (e.g. the Q, A and U).

The following is a design procedure for heat exchangers:

1. calculate the needed duty from the stream information.
   $$\mathbf{Q} = flow * cp * | t_{in} - t_{out} |$$
2. select a trial value for U, U_{ass}
3. calculate the mean temperature ΔT_m, from given input and output temperatures
4. calculate the required heat exchange area
   $$Q = U_{ass} * \mathbf{A} * \Delta T_m$$
5. make a heat-exchanger design: decide the geometry
6. calculate the overall resistance, U_{calc}, from the individual resistances
7. if the difference between U_{ass} and U_{calc} is too big, set U_{ass} to U_{calc}, go to 4 and start a new design cycle
8. calculate the pressure drops. If they are too large, go to 5 and change the geometry.

One of the difficulties in shell and tube design is to get a high heat transfer rate but at the same time low pressure drops in both streams. These are competing performance aspects: if the velocity of the fluids is increased (e.g. by more shell or tube passes), then the heat transfer rate also increases, but the pressure drop will be higher. The fluids lose pressure because of the longer flow lenghts. Moreover, more tube passes lead to more fluid flow reversals in the heads: every time the fluid leaves the tubes and enters the next tubes, pressure loss occurs.

3. A conceptual model

To get an understanding of heat exchanger design, the KADS methodology was used to build a conceptual model for this application domain [Schreiber, 1992]. KADS proposes a task, inference and a domain layer for modeling application-specific knowledge. We follow these layers in this section, and conclude with a discussion about the information generated during the design cycle.

3.1 Task and inference layer knowledge

On the task layer knowledge is present about the main tasks and subtasks of the application domain, and about the order in which these tasks should be performed (the control knowledge). On the inference layer the types of inputs and outputs of the non-decomposed tasks are modelled. This information can be represented in a graphical way in an inference structure (see figure 2).

Four main tasks are performed during the design process: Accept Requirements, Synthesis, Analysis and Evaluation. These tasks are discussed in the sequel. Below the control knowledge is presented in self-explanatory pseudo-code (note: the parameters are control parameters; the data input is not shown).

```
Accept-Requirements(ok-req)
if not (ok-req) then exit
ok-design := false
while not (ok-design)
```

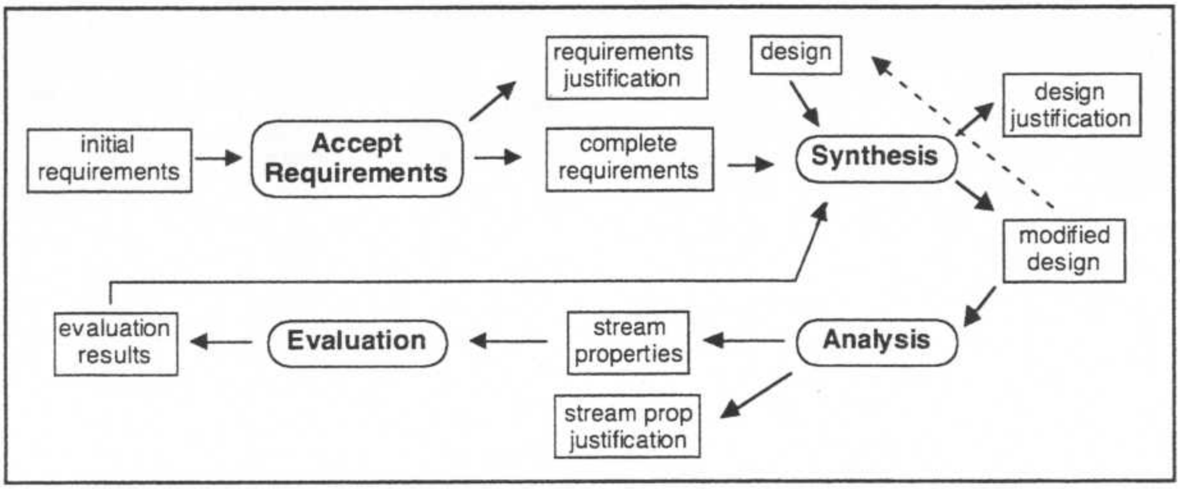

Figure 2. An inference structure for heat exchanger design

```
        Synthesis()
        Analysis()
        Evaluation(ok-design)
    end-while
```

Task Accept Requirements

During this task the initial requirements are checked for incorrect values (e.g. negative flows). Further, qualitative knowledge about the equations is used to determine if the requirements are over or underconstrained. In these cases the control parameter ok-req gets false, and the design cycle is terminated with a notification of the problem. Otherwhise ok-req gets true and the values of the dependent variables are used to get to a complete set of requirements. During this process, a 'requirements justification' is generated: a causal graph that shows how the values have been calculated (this depends on which variables were known in the initial requirements).

Task Synthesis

By synthesis we mean the determination of the structure of a design (e.g. its parts and their interconnection), the determination of the exogenous variables, and the setting of these variables. By restricting ourselves to shell and tube heat exchangers, the structure is fixed and only the latter two action are perfomed. So the synthesis task is now: how should the values of certain design variables be chosen ? If a design alternative does not satisfy the requirements: which design variables should be changed and how much ?

Task Analysis

During the analysis task, a numerical simulation is performed, to predict the influence of a design on the properties of the outgoing cold and hot streams. To predict the temperatures of the leaving streams first the partial heat transfer coefficients are calculated, then the overall heat transfer coefficient.

Task Evaluation

The simulation results of the previous task are compared with the requirements, and for every result an evaluation is given in terms of 'too high', 'too low', 'maximal', 'minimal' and 'ok'. If no requirements are violated then the control parameter ok-design gets true, otherwhise it remains false.

3.2 Domain layer knowledge

To perform the tasks described on the inference layer, domain-specific knowledge is needed. This type of knowledge is modelled in KADS on the domain layer.

For our domain we distinguished between four types of domain knowledge: 1. the relevant variables of the domain, 2. the qualitative relations and 3. the exact mathematical relations between these variables, and 4. synthesis knowledge. These knowledge types are explained below, followed by a discussion of their relations (see also figure 3).

Relevant Variables

We distinguish between the following types of variables: requirements, design and stream variables. The *requirements variables* describe the constraints that should be fulfilled by the design. In this case they include constraints on the properties of the incoming and outgoing streams, e.g. the input temperature, flow rate, (min.) pressure. A constraint that is deduced from stream requirements, is the needed heat transfer rate within the heat exchanger.

The *design variables* describe the geometry of the shell and tube, e.g. the number of tubes and tube passes, the diameter of the tubes. The *stream variables* describe all aspects of the streams needed for the design task. More information is needed about a stream inside a heat exchanger, than outside it. Outside the heat exchanger, a stream is described by its flow rate (kg/h), temperature, pressure, composition, and physical properties (e.g. viscosity, thermal conductivity). Inside also the partial heat transfer coefficient, the velocity through the tubes or around the tubes (m/s), the fouling factor, etc., are needed.

Many of the above-mentioned variables are related to each other. Relations exist between variables of the same type and of different types. For example:

- design variables relation: between the tube bundle diameter, the number of tubes, and the tube diameter
- stream variables relation: between the physical properties of a fluid and its temperature and pressure
- requirement variables relation: between the required duty and the required temperature difference of a stream.
- design and stream variables relation: the condition of the outgoing streams is dependent on the geometry of the design.

Numerical and Qualitative Relations

For the design task, the exact numerical relations are needed between the relevant variables. These relations are represented by a set of equations, and is called the *numerical model*.

However, an experienced designer uses besides the numerical model also his/her insight into the equations to understand the simulation results and to propose design improvements (e.g. why is the heat transfer rate so low ? what can I do about it ?). A qualitative model can be derived from the numerical model for this purpose. It reveales which variables are related to each other and how a change in a variable value will propagate to other variables (given information about which variables should not change).

For every pair of variables appearing in an equation, a relation is stored expressing the sign of the change of one of the variables, if the other is changing (other variables participating in the equation are assumed fixed). For example: to express the qualitative relations between the variables of the equation a + b = c, three relations are used: (QR a c +) (QR b c +) and (QR a b -).

Then, if a is rising and b is fixed, then one can deduce that c will rise. If c appears in other equations, the reasoning process can continue.

Synthesis Knowledge

Synthesis knowledge is needed to propose a first design, and to change the design alternative under consideration in a way that it will (hopefully) better satisfy the requirements specification. This type of knowledge is of a heuristic nature, and can best be modelled by if-then rules. Two examples:

```
if not-decided(tube-length) then suggest(tube-length,5)
if too-high(dPtf) and ok(Q)
then increase(tubes-per-pass) and keep(tube-passes)
```

Relation between knowledge types

As might be expected, there are relations between the four types of knowledge. First, the relevant variables determine the 'universe of discourse': all other knowledge types are expressed in terms of them. Next, the qualitative model is derived from the numerical model.

Finally, there are also relations between certain synthesis rules and the qualitative (and quantitative) model. For instance, the validity of the second synthesis rule above, can be explained by an investigation of the qualitative model (see figure 3). Thus, from the qualitative model synthesis rules can be deduced that propose the direction of change of a design variable.

3.3 Design process information

During the design process, several types of information are produced (see figure 2): information about requirements, design alternatives, simulation results (i.e. the properties of the leaving streams).

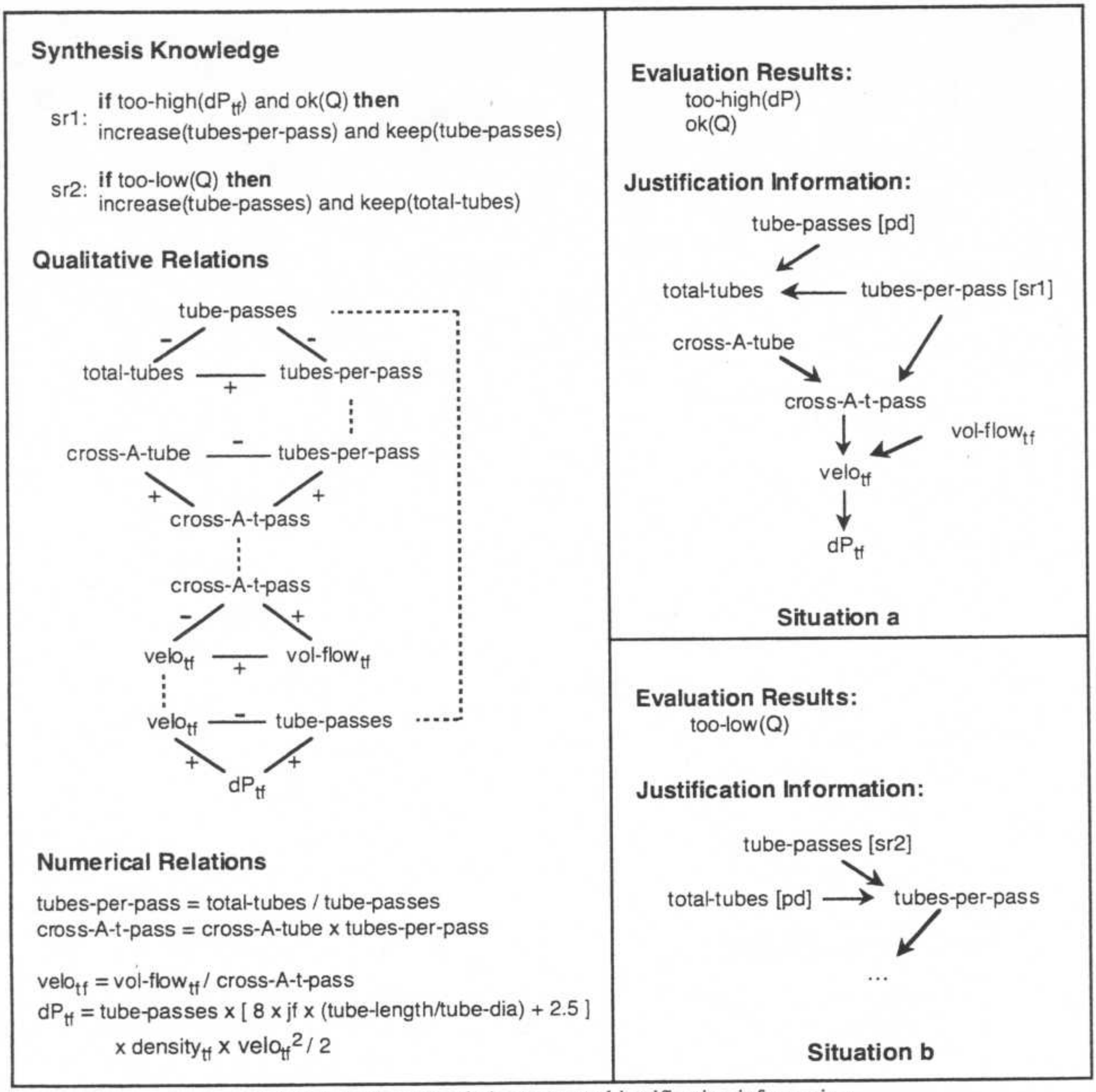

Figure 3. Design knowledge types and justification information

Besides, information is produced about the origin of these values: justification information. This information is important to remember, for the direction of the design process (e.g. the design alternatives that have been generated) and the final design can be explained by it.

One part of the justification information describes the origin of the exogenous variables: the user, a previous design, tables (e.g. for estimating the overall heat transfer coefficient), external routines (e.g. for calculating physical properties). The other part consists of a directed causal graph that reflects which variables were used to calculate the dependent variables. Thus it describes a 'causal ordering' among the variables ([Iwasaki and Simon, 1986; Iwasaki and Simon, 1994]).

The justification information may change at every design cycle. For instance, the overall heat transfer coefficient is first estimated by tables, afterwards it is calculated from the partial heat transfer coefficients. Another example (see figure 3, situation a): not always the same design variables are set; the number of tubes per pass can be set (e.g. by a synthesis rule), the number of tube passes taken the same as in the previous design, and from this information the total number of tubes can be calculated. But in another design cycle the number of total tubes and tube passes can be set, and the number of tubes per pass calculated (see figure 3, situation b).

4. The design system

In this section we will discuss the functionality of the design system, together with its architecture and knowledge representation choices. The system has been implemented in CLIPS, an OPS-style expert system shell with object-oriented features [Giarratano, 1993].

4.1. System functionality

The design system performs five main tasks: the four tasks identified in the conceptual model, and an explanation task. Three types of explanations are provided:

1. explain the use of a design modification proposal.
   This type of explanation is used to question a design heuristic. If the heuristic is grounded in the mathematical model, the qualitative and mathematical models can be used to justify its validity.
   Example. (S denotes the system, U the user)
   S: Proposal 1: increase tubes-per-pass and keep tube-passes
   U: Show heuristic 1
   S: Proposal 1 is derived by the following heuristic rule:
   "if too-high($dP_{tube\text{-}fluid}$) and ok(Q) then increase(tubes-per-pass) and keep(tube-passes)"
   U: Show QR 1
   S: Proposal 1 is justified by the following qualitative relations:
   $dP_{tube\text{-}fluid}$ is influenced positively by $velocity_{tube\text{-}fluid}$,
   $velocity_{tube\text{-}fluid}$ is influenced negatively by tubes-per-pass
   thus $dP_{tube\text{-}fluid}$ is influenced negatively by tubes-per-pass.
   U: Show equations 1
   S: Proposal 1 is justified by the following equations:
   $$dP_{tf} = \text{tube-passes} \times [\,8\ jf\ (\text{tube-length/tube-dia}) + 2.5] \times density_{tf} \times velo_{tf}^2 / 2$$
   $$velo_{tf} = \text{volumetric-flow}_{tf} / (\text{cross-area-tube} \times \text{tubes-per-pass})$$

2. explain the qualitative influences of two related variables.
   This type of questions can be used by the user to get an insight in the variable dependencies. The system uses the qualitative model for its answers.

3. explain the value of a variable.
   The causal graph associated with a design stage is used for this purpose. The origin of the value may be: the requirements specification, the user, tables, the previous design, a synthesis rule or the solving of an equation.

The design system performs under three modes: automatic, support and user mode. In the automatic mode, the user cannot intervene during the design process; given as input a requirements specification, the system repeatedly performs the synthesis, analysis and evaluation tasks, until a satisfactory design is found. At the end of the design process, the user can select one of the generated designs, and pose question type number 3.

In the support mode, the system uses its synthesis rules to propose a modification. The user can question the proposal (explanation of type 1), and accept it or not. The user can also use questions of type 2 to get an insight in the variables dependencies. In the user-mode, the system does not suggest any design modifications. The user can use questions of type 2 to come to a design.

4.2. System architecture and represenation choices

In figure 4 the modules of the design system are shown. The Main module is a control module. First it activates the Accept Requirements module. If its termination is succesful, the Synthesize, Analyse and Evaluate modules are activated. If the termination status of Evaluate is 'continue', then another cycle is initiated.

The Synthesize module is also a control module. Depending on the design mode it activates one or both of Suggest design and Accept design, followed by Assert Design. In Suggest design the system proposes a design modification; in Accept design the user can question the heuristics used and the qualitative and numerical models, and eventually accept a new design; in Assert Design first the dependent design variables are calculated and then a new design instance is created in the design space.

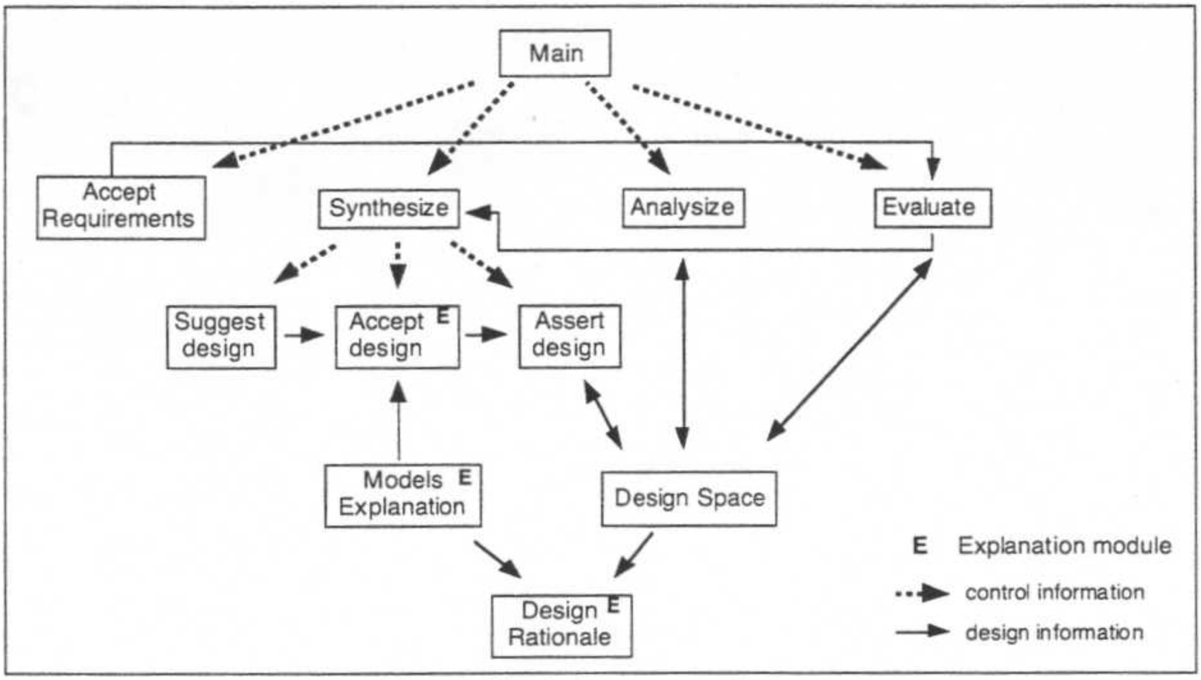

Figure 4. The design system architecture

The Analyze module creates two output stream instances. The values of these instances are the simulation results of the current design. The Evaluate module compares the requirements specification of the two output streams with the analysis results. For every comparation the result is 'ok', 'too high' , 'too low' 'max' and 'min'.

Module Model Explanation has an explicit representation of the numeric and direct qualitative relations used in the system. It also has rules for deducing indirect qualitative relations. Below an example of how a particular relation is represented.

```
Instance Heat-Transfer1
instance-of class Relation
attributes
  equation-name   "heat-transfer-across-surface"
  variables       Q, dT, A, oHTC
  equation        Q = dT * A * oHTC
  qual-relations  (Q,dT,+) (Q,A,+) (Q,oHTC,+)
                  (dT,A,-) (dT,oHTC,-) (A,oHTC,-)
```

Module Design Rationale posseses the reasoning potential for answering questions of type 3. For this task it requests information from the Design Space module, where all designs are stored, and Model Explanation (e.g. to show the equation that was used for a calculation step).

The Design Space module contains all information about the designs produced during the design process, their analysis and evaluation results. For every variable, not only its value is stored but also its origin. For example:

```
Instance Shell&Tube3
instance-of class Shell&Tube
attributes
  no-of-tubes          (300,user)
  no-of-tube-passes    (2,sr1)

Instance Stream-out3
instance-of Stream
attributes
  temperature     (30,eq3)
  pressure        (1.6,eq5)
```

5. Related work

Many QR-contribution have addressed the problem of qualitative model formulation, model selection, and dynamic simulation. In approaches like [Forbus, 1984], and [Catino e.a., 1991], the proposed models are based on physical processes, that describe the 'first principles' laws of physics and chemistry. Given a library of phenomena (the models), a scenario (system) description and certain assumptions (e.g. about the relative variable values), a reasoning mechanism is used to predict next qualitative states. For deducing the next qualitative step first the active processes and views are determined; then a causal graph describing how the variables influence each other and which variables are changing, is deduced; finally the information about the changing variables is used to describe the next state.

Our problem is different. We are not interested in deducing which processes take place, because we know that. Rather, we are interested in deducing how the geometry of an equipment (in this case a shell and tube) influences the *rate* in which processes take place. Thus, our simulation is numerical. Further, we don't use a qualitative model to predict new states, because steady-state simulation suffices for conceptual equipment design. Rather, we use the QM to explain the influences of certain design variables on the process rates (and other variables), and to suggest changes in the geometry.

Another difference is the source of the qualitative models. In the above-mentioned approaches, the right models for a certain situation are chosen from a library. In our case, their source are the numerical models. If they change, e.g. because a designer decides to describe a process in a different way, then the qualitative models would also change.

In [Iwasaki and Simon, 1986] the issue of causality between the variables of a device is discussed. Further, a method to come from a set of equations and a set of exogenous variables, to a 'causal ordering' between the variables is discussed. In our work, causal orderings are part of the justification information: they are generated when the dependent design variables and the outgoing stream properties are calculated.

In [Forbus and Whalley, 1992] a tutoring system for the analysis of thermodynamic cycles is discussed. The students propose certain aspects of a design, such as its structure and values for input variables, and the system deduces all concequences. Qualitative physics is used to check the values entered by the students, e.g. if a stream is to be cooled by a heat exchanger, then its final temperature should be less than its initial temperature. After the analysis step, the student can question the reason of a certain value, and the reason why an equation holds. The first question is comparable with our explanation of type 3 (see section 4). However, in this system no support is given for the synthesis task: what should the components of the system be ? how should the values of the input variables be chosen ?

In [Sgouros, 1993] a design system for the design of separation sequences in chemical processes, is described. Also in this research an integrated use of heuristic, qualitative and quantitative knowledge is advocated. The followed design cycle is more specific than the one presented in section 3, but the synthesis, analysis and evaluation tasks can be distinguished. In this approach qualitative models are used to generate design alternatives during a design cycle, and heuristic rules are used to choose one of these alternatives as the next current design. We use heuristic rules only to propose one design per design cycle, so in our case there is no need to choose among alternatives.

Acknowledgements

The research described in this paper was partly carried out at Akzo Nobel Engineering. The first author would like to thank Bert Ramaekers and Roel Murris for their support and the many fruitfull discussions about process design.

The authors wish also to thank Bert Bredeweg for his comments on an earlier version of this paper.

References

Catino, C. A., e.a. (1991). *Automatic generation of qualitative models of chemical process units*. Computers in Chemical Engineering 15(8): pp. 589-599.

Coulson, J. M., e.a. (1983). *Chemical Engineering, Volume 6:"An Introduction to Chemical Engineering Design"*. Chemical Engineering, Pergamon Press.

Forbus, K. D. (1984). *Qualitative Process Theory*. Artificial Intelligence 24: pp. 85-168.

Forbus, K. D. and B. Falkenhainer (1990). *Self-Explanatory Simulations: An integration of qualitative and quantitative knowledge*. In: Working Papers QR'90 Workshop pp. 1-13.

Forbus, K. D. and P. B. Whalley (1992). *Using qualitative physics to build articulate software for thermodynamics education*. In: IJCAI 1992 pp. 1175-1182.

Giarratano, J. C. (1993). *CLIPS User's Guide, version 6.0*, Report NASA, Lyndon B. Johnson Space Center.

Iwasaki, Y. and H. A. Simon (1986). *Causality in Device Behavior*. Artificial Intelligence 29: pp. 3-32.

Iwasaki, Y. and H. A. Simon (1994). *Causality and model abstraction*. Artificial Intelligence 67: pp. 143-194.

Schreiber, A. T. (1992). *The KADS approach to knowledge engineering. Editorial special issue*. Knowledge Acquisition 4(1): pp. 1-4.

Sgouros, N. (1993). *Representing Physical and Design Knowledge in Innovative Design*, Ph.D. Thesis, Northwestern University, Evanston, Illinois.

Yang, J., e.a. (1993). *Object-oriented knowledge based systems for process equipment selection*. Computers in Chemical Engineering 17(12): pp. 1181-1189.