USING GIFS IN THE ANALYSIS AND DESIGN OF PROCESS SYSTEMS

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A process system may be defined as an integrated combination of equipment which functions to produce one or more products, and possibly byproducts, by altering the physical and/or chemical nature of raw materials. Even though there is wide diversity in products produced, raw materials used, and equipment combinations employed, all process systems exhibit certain fundamental similarities. Characteristically, any process system may be subdivided into three operational phases. These are: preparation of raw materials, conversion to products, and recovery and purification. All three phases may not necessarily be included in a specific process system, nor is there always clear distinction among them. Still, there is universality in practice in that only a limited number of types of equipment are used to perform specific types of operations.

As an example of a relatively simple, but fairly typical, process system, consider the flow diagram for high-temperature isomerization reproduced in Figure 1. This is an operation performed in petroleum refining to improve the octane rating of certain gasoline constituents. It consists of a reactor for conversion, a flash drum and three distillation columns for recovery and purification, and several pieces of auxiliary

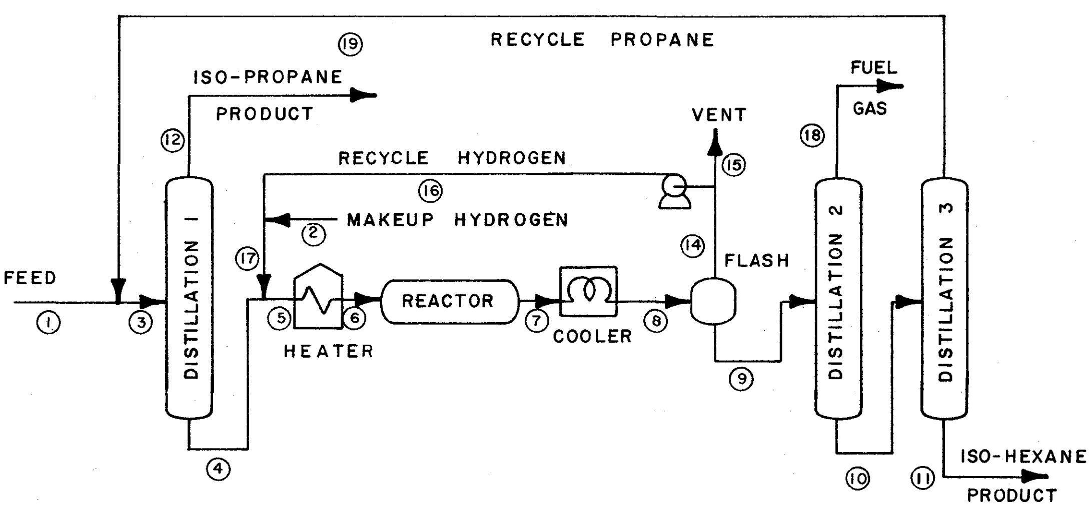

Figure 1. High-Temperature Isomerization

equipment. Distillation 1 also serves in preliminary preparation of the feed. Let us suppose that a unit similar to this is to be built for a particular refinery. Before individual pieces of equipment can be ordered or fabricated, it is necessary that their sizes and capacities be specified. This type of analysis is termed process design.

Prior to the general availability of computer methods, the process design engineer was forced to rely almost exclusively on information obtained from physical systems. Thus, if information about a similar unit, which was operating satisfactorily, was available, the design engineer merely gave the same or slightly modified specifications. For new processes, or processes for which comparison information was not available, he had to resort to scaleup from a pilot unit, construction of the pilot unit, in turn, being based on scaleup from a bench or laboratory unit. Thus, information required for construction of each process system was derived from a bench or laboratory model, through pilot unit, to production unit. This procedure is costly and time consuming. Further, the difficulties involved in experimenting with physical systems, especially of plant scale, all but prohibits investigation of anything more than minor design modifications.

As an alternate method of design, many computational methods are used. However, rigorous computations are too laborious for practical hand solution. As a consequence, only shortcut and approximate methods are used regularly, and their primary application is limited to supplementing plant and pilot information. Now that economical and reliable machine computations are readily available, lengthy, as well as complex, computational procedures are increasing in utility. Design is still ultimately based on comparison information, but this dependence is becoming less critical.

One of the many applications of computers in process design is in implementing the use of mathematical models. A mathematical model may be defined as a series of arithmetical operations performed to compute numerical values which represent certain performance characteristics of a physical system. Required input information are numerical values for design and operating conditions. A wide range in complexity is exhibited by the mathematical models which are programmed for computer solution. Some, such as for the mixing of two streams, are very simple, while others are very complex, requiring many hours of high-speed computer time for solution. The general concept, though, is the same. That is, given a numerical evaluation of operating and design conditions, the objective is to compute an estimate of performance characteristics for a corresponding physical system. Actually, this describes the simulation of a physical system using a mathematical model. An alternate type of mathematical model can be formulated for direct design. Accordingly, given numerical values for operating parameters and performance restrictions, numerical values for required design can be computed directly. Formulation of this type of model is normally much more difficult.

Many simulations for commonly used pieces of industrial equipment are being processed daily. However, this often requires theoretical isolation from the process system of which the piece of equipment is an integral part, and so may result in significant error. That is, the functional interrelationship of pieces of process equipment may be so significant, even with respect to the piece being studied, that gross errors in analysis may result when the effects of proposed modifications on the system are neglected. This is one of the primary motivations behind the development of Generalized Interrelated Flow Simulation, GIFS. That is, even more important than providing a convenient means of using preprogrammed mathematical models, GIFS provides a means of analyzing a process system as an integrated network.

The development of GIFS (Generalized Interrelated Flow Simulation) is based on study of a wide variety of industries. Representative among these are: petroleum refining, metals production, and manufacture of chemicals, pharmaceuticals, pigments, plastics, and pulp and paper. In essence, all of these represent special cases of continuous flow systems. Therefore, the design of GIFS is based not on the analysis of specific production systems, but rather, on the much broader scope of flow systems analysis in general.

The development of a generalized flow network method, which is easy to use as well as applicable to a wide variety of process systems, poses a number of difficulties. Outstanding among these is the ever-present possibility of system over or under specification. That is, there is a finite number of variables which, when fixed, completely determine a system, and all other pertinent variables can be computed. There is always the possibility that an engineer will attempt to set either more or fewer variables than are required for complete specification of a process system. In order to insure against this possibility, GIFS has been purposely restricted to analysis of cases which correspond to physical systems that are completely determined and which are not overspecified. Thus, GIFS is applicable only to the generation of a mathematical model to simulate the functioning of an entire integrated process system. No attempt has yet been made to incorporate direct design aspects in this model. In short, the method can be used only for the performance evaluation of a fixed process system at fixed operating conditions and with fixed feeds. This is really not a drastic limitation since design as well as optimization can be approached through multiple case studies.

In application, each system under consideration is represented as a network of interrelated stream flows. Figure 1 is an example. Each stream is identified by assigning to it a unique stream number as indicated. Numerical values which are used to describe the nature of a stream are termed stream properties. Stream properties include total flow rate, composition, temperature, pressure, heat content, and phase state. Restrictive relationships among streams, such as are simulated by preprogrammed mathematical models for specific types of process equipment, are indicated by what is termed unit computations. Examples of unit computations include the simulation of process equipment, such as reactors, distillation columns, heat exchangers, etc., as well as factors which have no direct equipment counterparts (pressure drops in lines and ambient heat exchange). The currently available library includes 21 unit computations. These are summarized in Table 1. Complete descriptions are given in the GIFS user's manual.* They represent a collection which is basic in nature and highly versatile. Further, GIFS is constructed so as not to be limited to the library of unit computations available at any one time. At present, four additional unit computations are being prepared for inclusion in the library, and others can be added as specific needs arise.

Figure 2 is a reproduction of one page of the input data sheet which describes Figure 1 in terms of unit computations. Each unit computation is specified by giving the unit computation type, associated stream number or numbers, and arguments if any. A unit computation number is included for identification only. It is usually convenient to number unit computations sequentially. The first unit computation in Figure 2 indicates the addition of streams 1 and 19 to obtain stream 3. The unit computation type is STAD (Stream Add), and the associated stream numbers are 1, 19, and 3. The second unit computation indicates the function of distillation column number 1, the associated streams being 3, 12, and 4. The unit computation used is CRSEP (Component Ratio Separation). This is an approximate simulation of a distillation column which requires, as arguments, component recoveries for all components present in the feed (ratio of component flow rate recovered in the overhead product, stream 12, to component flow rate in the feed stream, stream 3). Since there are eleven components for the illustrative system, values for eleven arguments are entered. Additional unit computations necessary to describe the entire system are entered sequentially. Detailed information on the preparation of input data sheets is contained in the user's manual.*

The objective of each computation is an evaluation of all interrelated stream properties. These are computed as a function of the properties of the given feed streams. Each system is computed as an integrated network and in a manner which satisfies fundamental material balance relationships as well as the restrictions defined by the specified unit computations. Systems are normally non-linear, and a method of solution by iteration is employed. As an example of a computer output, just one portion of the report for the illustrative example is reproduced in Figure 3. This is the portion which describes computed properties for stream 9.

*GIFS, Generalized Interrelated Flow Simulation, user's manual is available through any SBC office or local sales representative.

SBC

GIFS
UNIT COMPUTATIONS

UNIT COMPUTATION NO. (01–03)	TYPE (11–20)	STREAM 1st (21–23)	STREAM 2nd (24–26)	STREAM 3rd (27–29)	ARGUMENT 1st (31–40)	ARGUMENT 2nd (41–50)	ARGUMENT 3rd (51–60)	ARGUMENT 4th (61–70)
1	STRD	1	19	3				
2	CRSEP	3	12	4	1.	1.	1.	1.
					1.	1.	.97	.01
					0.	0.	0.	
3	BPT	4						
4	STQ	4						
5	STRD	4	17	5				
6	QFLSH	5						
7	STQ	5						
8	STFQ	5	6					
9	TSET	6			750.			
10	TFLSH	6						
11	STQ	6						
12	REACT	6	7		2.	9.	8.	.63
					.003	.008	.003	.002
					.01	.879	-1.	.005
					.001	2.	3.	4.
					5.	6.	7.	8.
					9.	10.	10.	10.
					.21	.008	.008	.033

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Figure 2. Sample Input Data Sheet

STREAM 9 FLASH LIQ

COMPONENT NO.	NAME	TOTAL FLOW MOLES/HR.	MOLE FR.	LBS./HR.	WT. FR.	VAPOR MOLES/HR.	LIQUID MOLES/HR.
1	H2	1.2926	0.0139	2.5853	0.0003	0.	1.2926
2	C1	0.3115	0.0033	4.9845	0.0007	0.	0.3115
3	C2	0.1001	0.0011	3.0124	0.0004	0.	0.1001
4	C3	0.0682	0.0007	3.0062	0.0004	0.	0.0682
5	I-C4	0.0472	0.0005	2.7415	0.0004	0.	0.0472
6	N-C4	0.2389	0.0026	13.8804	0.0018	0.	0.2389
7	I-C5	22.2530	0.2389	1604.4429	0.2125	0.	22.2530
8	N-C5	3.4096	0.0366	245.8286	0.0326	0.	3.4096
9	I-C6	18.3820	0.1973	1584.5274	0.2098	0.	18.3820
10	N-C6	44.9652	0.4827	3875.9987	0.5133	0.	44.9652
11	C7+	2.0943	0.0225	209.8512	0.0278	0.	2.0943
	TOTALS	93.1626	1.0000	7550.8590	1.0000	0.	93.1626

PRESSURE	300.00	PSIA.	TEMPERATURE	120.00	DEG. F.
VAPOR FLOW	0.	M CU. FT./HR.	LIQUID FLOW	25.04	GPM
(Z = 1.0)	0.	M STD. CU. FT./HR.			
HEAT CONTENT	-0.	MM BTU/HR.	FRACTION VAPOR	0.	

Figure 3. Computer Report

Table 1

Unit Computations Summary

Title	Type	Streams	Arguments
Stream Add	STAD	ST1 ST2 ST3	
Stream Subtract and Zero	STSBZ	ST1 ST2 ST3	
Stream Split	SPLT	ST1 ST2 ST3	F12
Stream Equate	STEQ	ST1 ST2	
Stream Zero	STZ	ST	
Temperature Add	TAD	ST	DT
Heat Add	QAD	ST	DQ
Pressure Add	PAD	ST	DP
Temperature Set	TSET	ST	T
Heat Set	QSET	ST	Q
Pressure Set	PSET	ST	P
Vapor Ratio Set	RSET	ST	R
Bubble Point	BPT	ST	
Dew Point	DPT	ST	
Isothermal Flash	TFLSH	ST	
Adiabatic Flash	QFLSH	ST	
Constant R Flash	RFLSH	ST	
Stream Heat	STQ	ST	
Equilibrium Separation	EQSEP	ST1 ST2 ST3	
Component R Separation	CRSEP	ST1 ST2 ST3	R1 R2 --- ---- RN
Reactor	REACT	ST1 ST2	NR NC1 NK1 CNV1 S1 ---------- SNC1 C1 ---------- CNC1 --------- CNCNR

GIFS has been developed, and is now being offered, as one of SBC's preprogrammed computer services. Characteristics of these services include accurate, inexpensive, and rapid processing for a wide variety of problems, use of convenient input data sheets, and the presentation of computed values in clear, comprehensive reports. Cases which have been processed to date represent applications in such fields as petroleum refining, inorganic and organic chemicals manufacture, and pulp and paper production. These have been processed in a routine manner, and have not indicated any unforseen complications in the approach or the computer implementation. From all indications, companies who are using the service are highly satisfied, and expect to continue using it. Future developmental efforts will depend on industrial response. SBC is already contemplating the implementation of a number of additional features.

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