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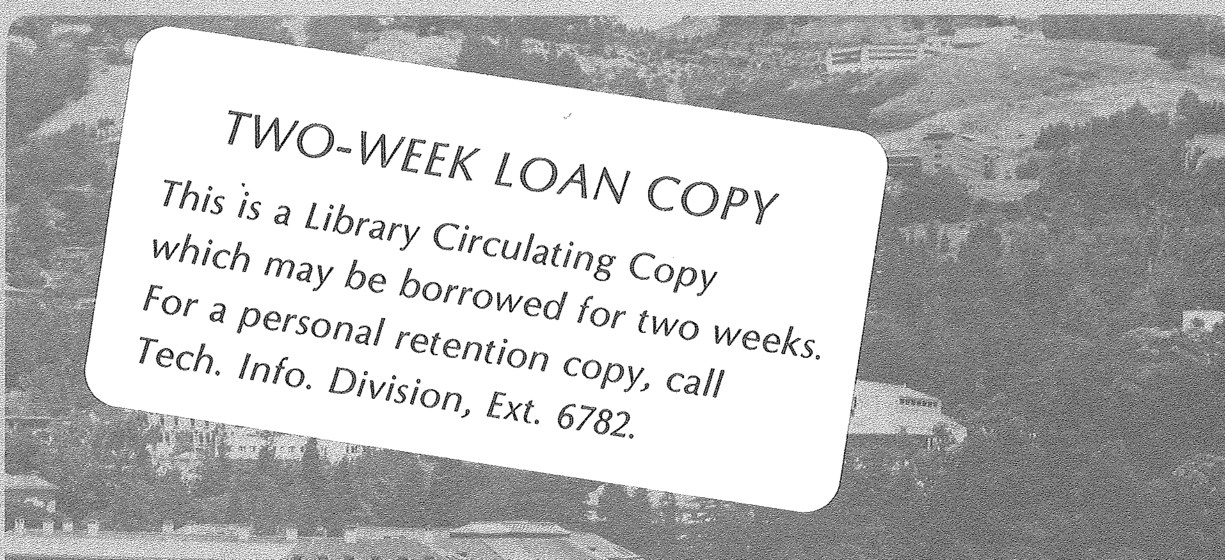
MATERIAL-FLOW DATA STRUCTURES AS A BASIS FOR ENERGY INFORMATION SYSTEM DESIGN

V. V. Krishnan and D. F. Cahn

April 1980



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In efforts aimed at information system design to assist national energy decisionmaking, we have analyzed the U.S. petroleum supply and distribution system. The overriding goal was to develop data structures conducive to information system design; this led us to emphasize methodological uniformity and generalizability. Quantized petroleum flows among restricted channels in the distribution net form the basis of the data structure. The resultant vectorial representations provide a direct link between conceptual models of system function and information system implementations to capture them. Simultaneously, they ease otherwise difficult problems such as data validation and error isolation.

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The utility of an information system in supporting decisionmaking depends heavily on the adequacy with which relationships among the data of interest are represented. If queries of interest cannot be answered because required data are missing or because data comparisons or combinations cannot be constructed as needed, the decisionmakers must look elsewhere for assistance. Similarly, the configuration of the data structure influences the ease with which new data can be validated, and thus substantially affects the integrity and credibility of the system.

As one phase of an effort aimed at formulation of advanced information systems to support national energy policy decisions, we have conducted an analysis of the U.S. petroleum supply and distribution system. The focus has been on identification of major system relationships and information structures appropriate to represent them. Insofar as practical, we have stressed uniform and general representations, with the notion of facilitating the subsequent information system design. Uniformity is a desirable trait both in spanning the petroleum domain and in extension to other energy modalities. In the past 1 , energy data systems have served ad hoc regulatory purposes, and an overall system view of the existing data pool has been lacking.

CHARACTERISTICS OF THE MODEL

The primary concepts behind our petroleum supply model are drawn from engineering control theory [2]. Between crude oil production or importation and refined product consumption, petroleum passes through a set of interconnected nodes. The nodal interconnections are vectorial, and provide an explicitly restricted signal channel between, say, processing modifications (refining, etc.) in one node and storage or transportation in the next. By isolation of those nodes at which identity and volume changes can occur (such as refining) from those at which material identity and volume are expected to be conserved (such as transportation), it is possible to select generic data nodes at which product monitoring can give validation crosschecks. There have been past efforts in this direction, most notably the Project Independence Evaluation Study [3], but the orientations of these have been different from ours: while we are concerned with clarification of a specific kind of data relationship (material supply flows), and with identification of common denominators and uniform coupling equations throughout the system, the previous models have attempted to model demand and its influencing factors as well as supplies. The broader orientation of these previous models has necessitated a more macroscopic data view than ours, and has made it difficult to address important information system capabilities such as data validation and error isolation.

Oil in the system is considered to exist as a set of quantized units or "packets". Each oil packet has associated with it a set of attributes that, when organized into a vector, provides a description of the current "state" of the packet sufficient to characterize it from all aspects. In particular, the attribute set must be sufficient to answer expected classes of queries concerning, for example, types (by chemical composition, tier, etc.) of petroleum in the system, present locations and volumes of oil or petroleum products, volume of oil (or product) in storage and volume in transit, geographic source and destination, transportation medium, and current price at any given stage. Ideally, the packets represent individual oil shipments or consignments, although the model is robust over aggregation, and the packets could just as easily represent monthly corporate totals. The primary consideration is one of desired usage rather than any anomaly of the data structure: the packets and attributes together determine the resolution grain of the model, and thus the combinatorial questions it can answer. We cannot hope reliably to answer questions dealing with daily flows among individual refineries if we have only monthly data collected on an aggregate corporate basis. Since the packet view applies over many aggregation levels and control volumes, we preserve generality by basing our system on it.

A. Functional Stages and Material Phases

The petroleum flow model (Figure 1) is predicated on a control boundary surrounding the U.S. and is organized at its most general level into three stages - Supply, Processing and Consumption - with flows from one stage driving the next. We have emphasized "consumption" rather than "demand" to indicate that the model represents actual use of petroleum rather than predictions. The three major stages are connected by unidirectional transportation links (denoted by thick arrows). As Figure 1 shows, total crude oil available for domestic use in the U.S. is the sum of domestically produced crude and the crude oil imported from abroad minus the amount of crude oil exported.

It is useful also to segragate crude oil and oil products into quasi-independent material phases, as denoted by the horizontal brackets at the top of Figure 1. The connecting link, the refining process, normally requires a predictive model. However, given the product latitude available in distillation and the other refining processes, and the responsiveness of refining product decisions to economic considerations as well as those of pure chemical stoichiometry, refining models adequate for material accounting purposes are not presently available. By accounting for crude oil and petroleum products separately, one can sidestep the relative unpredictability of the refining process and preserve the accuracy and usefulness of the data support functions of the model. The pre-refining material, crude oil, is traced until its consumption at the refinery inlet, and the post-refining materials, petroleum products, are traced from their source at the refinery outlet.

Imported oil is traced only from the point at which it crosses the U.S. control volume and goes into storage at a U.S. port of entry, and exported oil only to storage at U.S. port of export. One might reasonably extend this model to the country of origin in the case of imports and to the country of destination in the case of exports, but this was not done in the present model because, on an ongoing basis,

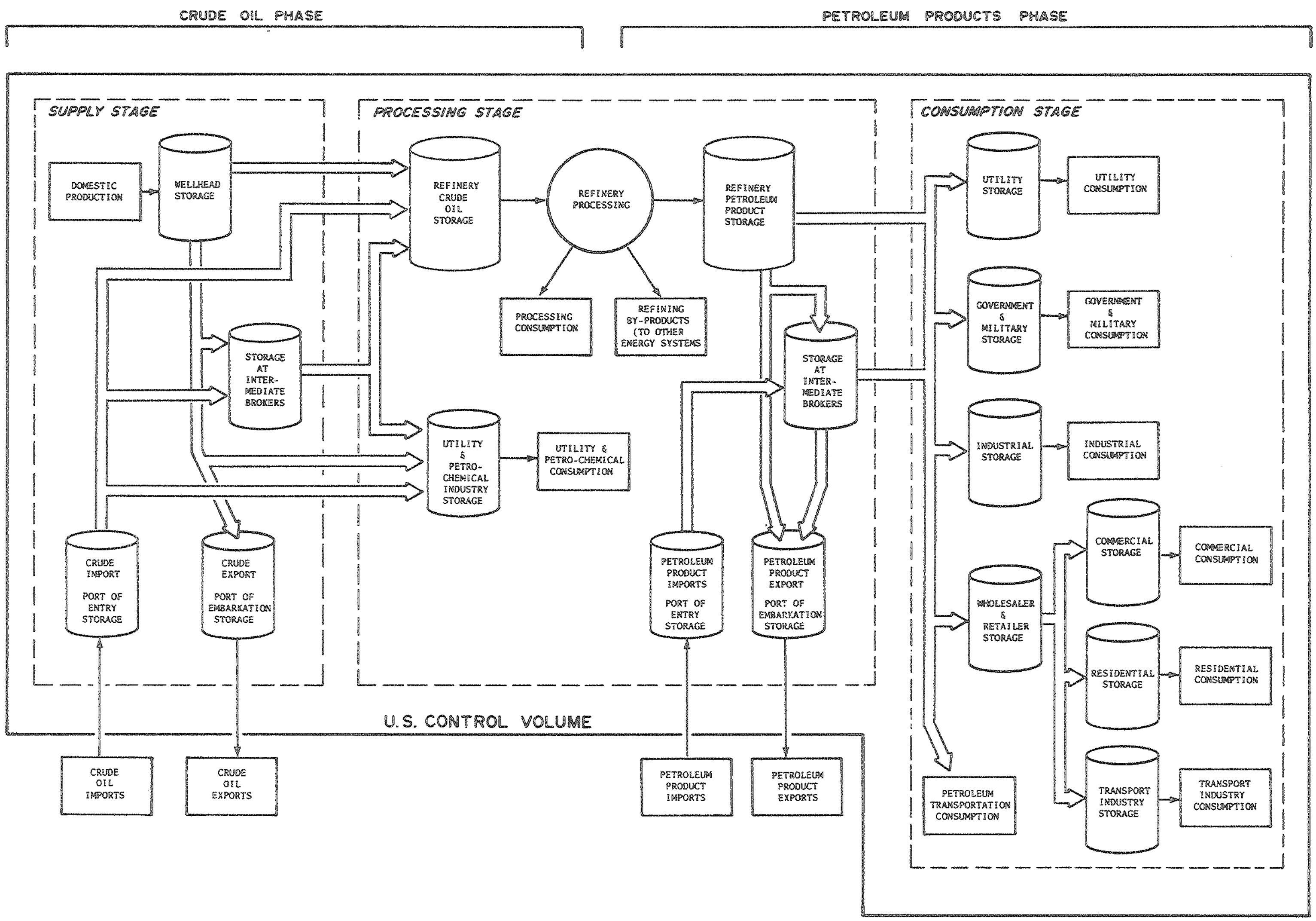

FIGURE 1. Major flows in the U.S. petroleum system. Cylinders denote matrices of storage facilities, rectangles denote material sources and sinks, circles denote material transformation sites, thick arrows denote physical transportation. Heavy boundary indicates control volume bound for U.S.; brackets and dotted lines denote material phases and processing stages as marked.

the requisite transportation data may not be obtainable within the authority bounds of U.S. agencies unless the oil is transported by U.S.-based carriers, and thus may be expected to be generally incomplete.

Each storage element (cylinders) and each transportation element (thick arrows) is in fact composed of a data matrix containing specific instances of the generalized unit named (or connecting named elements, in the case of the transportation links). The cylinder representing "Wellhead Storage," for instance, is a matrix containing data on all the storage facilities at well sites throughout the country; for each such site, information on volume, location, owner, etc., is organized, for each distinct type of crude oil kept separately in storage, into a vectorial representation. The matrix ensemble of these "attribute vectors" gives a picture of the entire wellhead storage of crude presently within the country, regardless of location; i.e., wellhead storage is organized into a generic class.

Crude oil can flow from wellhead storage to refineries, to intermediate brokerage and resale, to export, or to the utilities and petrochemical industry; by isolating into generic classes the storage that crude may undergo (as described above), the number of general interaction path types connecting elements can be drastically limited, with obvious advantages for information system design. The actual number of site-to-site paths is much larger, but organizing them on a generalized basis allows the interaction links themselves (in this case involving physical transport) to be represented in a homogeneous matrix covering the entire country. (Source and destination simply become two of the attribute data values associated uniformly with each interaction link.) The uniformity of the representation is, of course, a key requirement in applying computer information processing procedures advantageously.

For any block, material inflows and outflows take place unidirectionally, as shown by the arrows. A summation over all flows so represented provides a continuity equation for the block, and, barring sourcing or consumption within the block (intentionally isolated throughout the model and restricted to the rectangular blocks shown in Figure 1), should give a conclusive picture of all state changes affecting the block. This continuity principle, carried forth over the entire system, provides a powerful mechanism for data validation.

In the data model, each class of unit (for example, wellhead storage) is represented by a matrix whose elements are subunits of the class. The size of the subunits determines the resolution or grain size. For example, an element of the matrix representing wellhead storage could represent all such storage belonging to a company, the portion located within a specified state, a specified tank farm, or even a single tank. The usefulness of the model (and perhaps the cost of collecting and maintaining the data) will increase with increasing resolution; however, the properties of the model, as described below, are independent of grain size. In particular, the form of a data transformation representing oil flow (or representing a purely financial transaction) is independent of the level of aggregation.

B. Packet Attribute Vectors

Each flow packet in the system is represented by a vector of attribute values describing its contents. The twelve variables defined below are sufficient to characterize a packet in any stage or phase of the system. Generally, the attribures reference dimensions of the element blocks (to be presented in Section D below), as well as addressing values within the transiton vectors.

$$STATE_{packet} = f(Q,A,T,P,I,J,K,W,C,D_I,D_F,x)$$

Q: Volume of crude oil or product being transported or stored.

A: Chemical composition (sweet/sour, light/heavy, originating oil field [4], etc.).

T: Oil price-tier per the U.S. Federal price-tiering structure.

P: Price per unit volume actually paid for the packet by the company reporting the transaction.

I,J: Geographical regions(state, zip, PAD region [3], etc.) associated with either transportation or storage of a given packet of oil. When the reported datum refers to an oil packet in transit, I represents the origin of the shipment and J represents the destination. When the reported transaction concerns oil in storage, I represents the location of the storage facility and there is no entry for J.

K: Transportation mode used for a particular shipment. There are five major modes of transport currently in use for oil: pipelines, waterways, coastal tankers, railroads and trucks.

W: Owner of the packet. It is entirely possible (1) that neither shipper (I), receiver (J), nor transportation agent (K) may own the oil they are handling, and (2) that an oil packet can change hands without being moved at all. Further, (3) there is considerable latitude in the reporting of ownership transactions (for example, with a shipper reporting a packet sold as of date of order receipt and a receiver reporting it purchased as of date of payment, possibly two months later). Given these situations, it is necessary to consider packet ownership as distinct from its current location or destination.

C: Consignee of the packet. Necessary for the same reaons as W. Further, since a packet may go through several sets of (I,J,K) before delivery to its ultimate consignee C, there is a further impetus to defining a separate variable.

D_I,D_F: Initial and final dates of packet transition across a given port. If, for example, it takes three days to pump a 200,000 barrel gasoline consignment into tank cars for shipment from refiner I to distributor J, than I's outlet port is involved iwth the shipment from (D_I) to

($D_F = D_I + 3$). Since, especially in the case of synchronous reporting intervals for cumulative totals at various facilities, this represents a reporting error band, it is useful to know what state each shipment is in while it is in transition. These dates are also useful in verifying identity of shipments being traced.

x: A local shipment identifying index. This need not be assigned systemwide (which would be burdensome), but merely serves to match up a release vent at the outlet of one block with an acceptance event at the inlet of the block immediately downstream. Typically, a shipping document or invoice number.

C. Facility Attribute Vectors

Several secondary attributes are associated with the physical facilities that handle the oil, and act as background constraints on the packet variables. Since these change only infrequently, it makes sense to store them in a secondary information space. These variables are mostly transportation-related, but at least one, Capacity (CP), is relevent to both transportation and storage. In both flow states, CP gives the maximum storage available at the facility. By contrast, Q, the packet volume, represents volume actually being held. Emergency decisionmaking, in particular, is sensitive to such data as reserve refining and pipeline capacity, i.e., (CP-Q), and dictates inclusion of secondary data of this sort.

$$STATE_{facility} = g(D,TC,t,CY,CP)$$

D: Distance from I to J using mode K.

TC: Tariff cost data for transportation mode K from location I to location J.

t: Time taken for transporting crude oil or petroleum product from I to J using mode K.

CY: This attribute represents the average cycle time for transportation mode K. for example, the turnaround time for a ship.

CP: Facility capacity. For storage facilities, the maximum volume or mass storable. For transportation, the total contained n a pipeline, truck fleet, etc., when operating at optimum efficiency. Note that, since products generally cannot be mixed, this variable in fact must be quantized: for example, for a tank farm, CP is really a sum of the capacities of individual tanks, any of which can contain only a single homogeneous product at any moment. Thus, CP has a bearing on primary attribute A, and there is, instantaneously, a maximum CP for every chemical type A.

D. Structural Element Blocks

The process model of Figure 1 can be further subdivided into blocks (Figures 2 and 3), and the blocks then "plugged" together via explicitly constrained interconnections ("ports"), as shown in Figure 4. Material flow between blocks is universally characterized as occurring in packet units, and each packet is completely specified by its associated attribute vector. The blocks themselves are data matrices, and contain cumulative information on material in the system organized by packet vector.

Five system blocks, depicted in generalized and sample form in Figure 2, are sufficient to characrerize all elements in the system model. Material passes through each block in a unique direction (from acceptance (or inlet) port to release (or outlet) port), and between blocks only through specified port-to-port contacts. This flow channeling has several ramifications:

(1) Transitions are isolated to the port interface, and a packet is unitized once it has entered a block and cleared the inlet port. This allows storage of single values for each volume Q held within the system block, rather than the subarrays that would be needed if transitions were allowed to propagate.

Transition isolation establishes a useful error constraint on the system: since no state modifications are allowed internally in the blocks, all material losses and gains, ownership changes, etc., are accounted as sequential transition vector events. Since no valid modifications are allowed internally, any state changes that are not accountable as interface events are immediately detectable as anomalies. such formalization of transition events is beneficial in tracking two party transfers, and becomes critical when the transfers are chained, as is common in the industry: oil may be sold from I to K, and subsequently from K to J, rather than from I to J with K merely as a transfer agent. In this case, the oil delivered by K to J may be physically distinct from the oil received by K from I.

(2) Incrementation events affecting system blocks may be handled sequentially. Since each vectorial packet, regardless of source or destination (which are variables specified in the attribute vector), passes between blocks in a channel restricted to be only one packet wide, inputs to and outputs from any block in the system affect the block contents one packet at a time. With transitions restricted to the port connections, the internal states of the blocks are subject to a sequence of controlled modifications and are well defined at any instant. By contrast, if the ports were unrestricted, internal state modification would be continuous and very hard to trace.

(3) Since source (I), destination (J), and other variables in the input and output packet vectors directly address the particular entries in the block matrix that are affected by the packet, and since incrementation events are sequential, the states of the block matrix entries are static except where instantaneously addressed. Thus, stepwise tracing of the effects of particular shipments or other modifications is straightforward: if, for example, some precipitous event happens whose significance is only

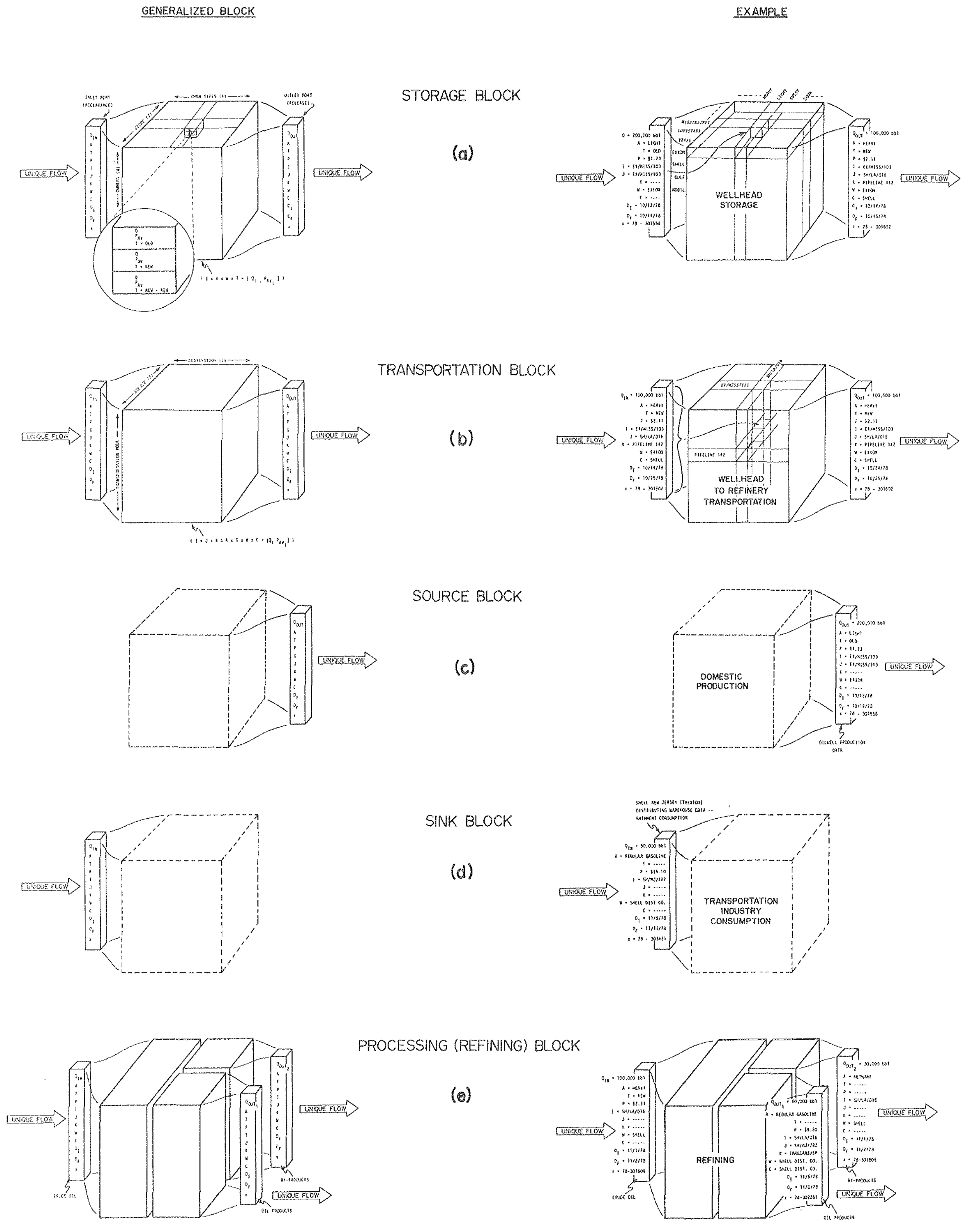

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FIGURE 2. Matrix block representations for model elements. Generalized forms and examples for each of the five block types that, together, completely represent all portions of the petroleum model:(a)- Storage; (b)- Transportation; (c)- Source; (d)- Sink; (e)- Processing (refining). Vectorial packet input/outputs depicted.

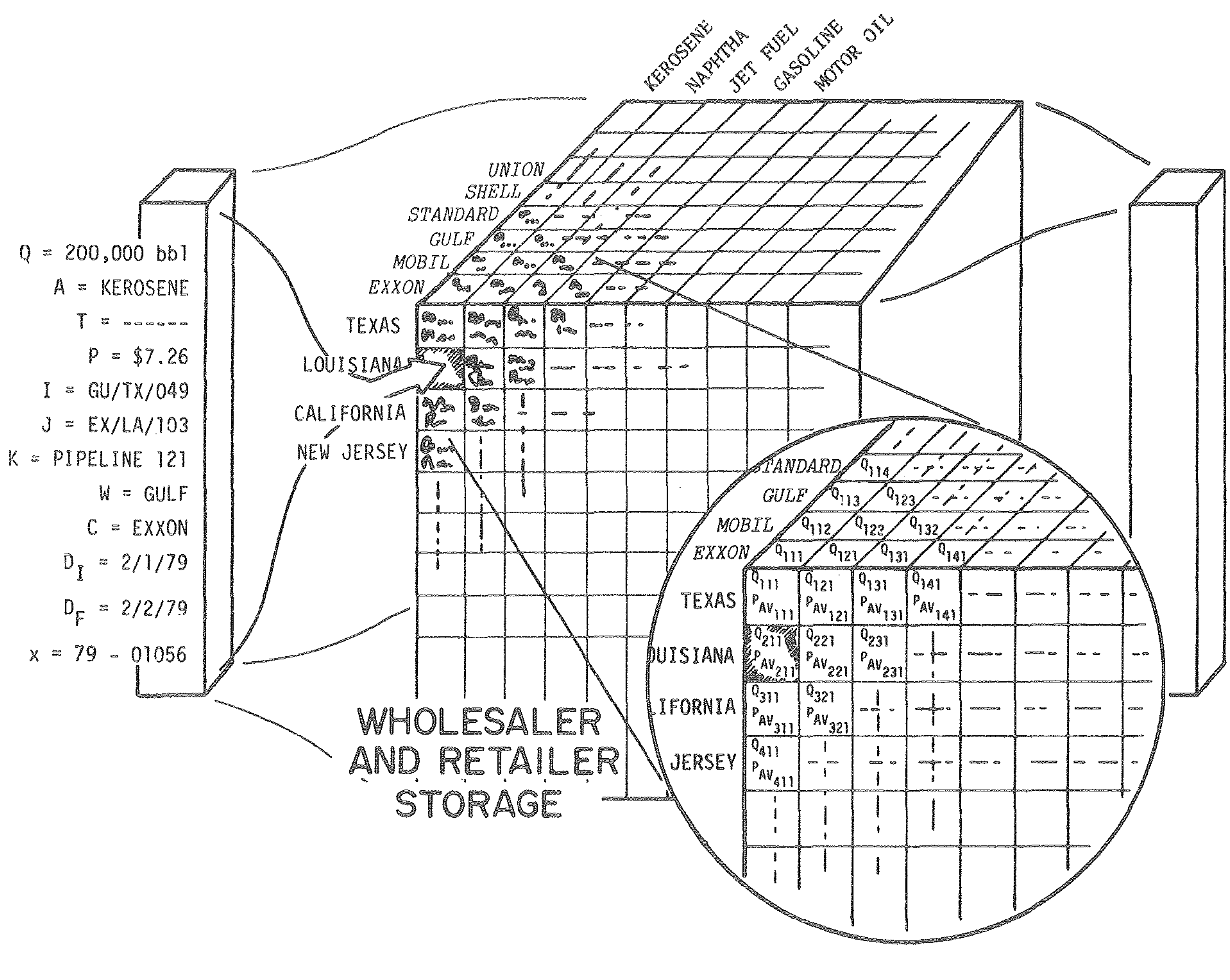

FIGURE 3. Effects of a petroleum packet received through the inlet port of a block. Received packet is routed to the appropriate element of the storage matrix, and modifies its entries for volume Q and average price P_{AV} accordingly.

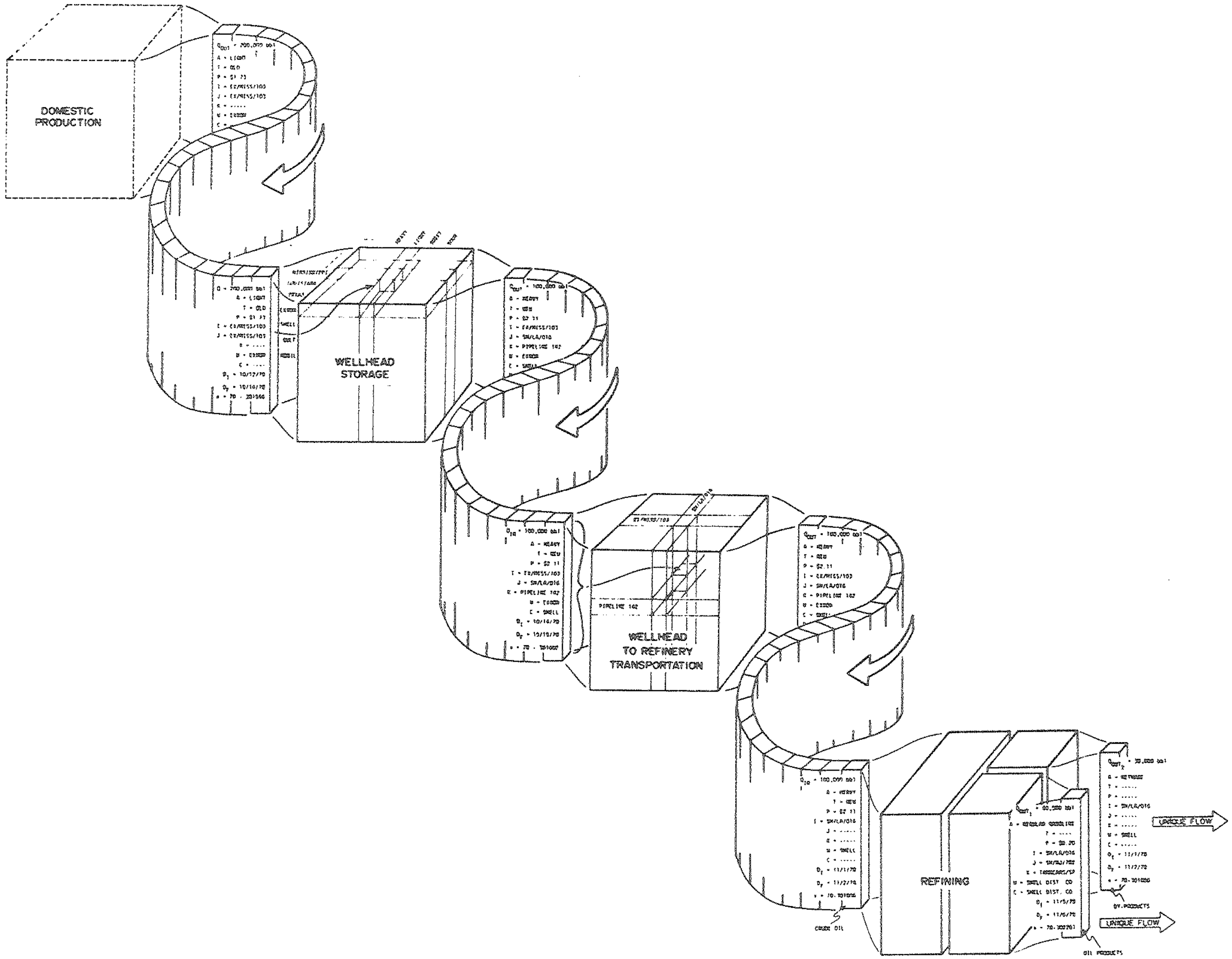

FIGURE 4. Sequential flow through connected blocks representing a portion of the Figure 2 model. Vectorial packets leaving one block flow through a sequential channel restricted to be one unit wide and impinge on the next block downstream. Such incrementation events, properly addressed to specific matrix elements within the blocks, are the only ones allowed to modify the block contents.

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recognized later, it is possible to recreate the initial system state and step through the subsequent modification events one at a time, thus illustrating, in sequence, the effects of the instantaneous modifications on various parts of the system, and thereby aiding analysis. Such "stop motion" or "instant replay" tracing would be far more difficult (if not impossible) if many modifications were allowed to occur simultaneously as would be the case without the flow restriction.

Similarly, a "sentinel" [5] may be established looking for, say, all flows of gasoline to and from Exxon facilities in New Jersey; establishment of such a sentinel (which could provide, for example, lists of suppliers and customers for Exxon's New Jersey gasoline facilities, together with their volumes added or used, plotted against time) woud entail merely accessing the single appropriate point in the refinery product storage matrix and tallying all modifications to it as they happen.

Internally, the blocks themselves are data matrices, as shown by example in Figure 3. For the refinery petroleum product storage block shown in the figure, as for other blocks throughout the system, certain of the transition vector variables address necessarily isolated repositories of product. In all cases, though, the primary variables of interest are the volume (Q) of product on hand and the average price (Pav) paid for that volume. If, for example, an Exxon wholesaler in Metairie, Louisiana, receives 200,000 barrels of kerosene from a Gulf refinery in Galveston, Texas, and puts it in an on-site tank already containing kerosene (which he must do because the products cannot be mixed), then this 200,000 barrels adds selectively to Exxon's kerosene supply in Louisiana. An inlet vector representing the reduced volume impinges on the product storage block and is directed exclusively to cell 211, where it modifies Q_{211} and Pav_{211} according to some appropriate set of incrementation equations such as those below:

Typical generalized node modification equations:

$$Q_{final}(A,I,W,T) = Q_{initial}(A,I,W,T) + \sum_{\tau} q_{in}(A,I,W,T) - \sum_{\tau} q_{out}(A,I,W,T)$$

$$P_{av_{final}}(A,I,W,T) = \frac{(P_{av_{initial}} * Q_{initial}) + \sum_{\tau}(p_{in} * q_{in}) - \sum_{\tau}(P_{av_{final}} * q_{out})}{Q_{final}}$$

where τ is a predetermined modification interval (which, in fact, may be set short enough to restrict modification events to occur singly), and outlet flows are considered to occur at the average purchase price rather than actual selling price, so that Pav_{final} will reflect average price paid for the cumulated material at each successive stage.

Sample Application (see Figure 3):

- Initial conditions:

$$Q_{211_{initial}}\text{ (kerosene,EX/LA/103,EXXON,--)} = 400{,}000 \text{ bbl.}$$

$$Pav_{211_{initial}}\text{ (kerosene,EX/LA/103,EXXON,--)} = \$6.57$$

- Modification effects:

$$Q_{211_{final}}\text{ (kerosene,EX/LA/103,EXXON,--)} = 400{,}000 + 200{,}000$$

$$= 600{,}000 \text{ bbl.}$$

$$Pav_{211_{final}}\text{ (kerosene,EX/LA/103,EXXON,--)} =$$

$$= \frac{6.57 * 400{,}000) + (7.26 * 200{,}000)}{600{,}000} = \$6.80$$

The five generalized block types naturally form three sub groups: material-conservative, material-nonconservative, and hybrid. In the ideal case, the storage and transportation blocks are expected to conserve material. Material enters, is routed to an appropriate matrix element and sums with the element's previous contents. In a similar manner, material flowing out of the block is drained only from the appropriate matrix element. Transactions can occur on material without generating its physical movement; however, even when the transaction is just an assignment of some volume between branches of a company (without even an exchange of dollars), a modification event has taken place that will be visible to the model as a state change (as long as the data is reported). Specifically, a volume (Q) of some type (A), tier (T), etc., of material has changed owner (W); the separate reports for the Q sent from the old owner W_i to the new owner W_j, and received by the new owner W_j from the old owner W_i, should exist just as if a physical shipment had occurred, and would corroborate each other in referencing a specific packet vector.

The second subgroup contains blocks (4) and (5), the sources and sinks. These are material non-conservative in that they represent points at which material enters or disappears from the system. In fact, the material does not actually appear or disappear, but, as noted previously in the presentation of Figure 1, we must define explicit boundaries for the system being modelled to exclude data that we cannot obtain. Thus, for example, we treat crude oil imports as a source element; we cannot be sure of data reported by foreign entities, and consider the source outlet vector at the U.S. border (i.e., U.S. Bureau of Customs Import data) as a point at which material simply appears. Similarly, gasoline consumed in, say, the transportation industry, is simply removed from the system at the outlet from the last point to which we trace it (in the present model, the wholesale distributor). As a final example, gaseous refinery by-products leave the oil reporting system and (presumably) enter the natural gas or some other reporting system. Here, we really have a transportation or storage block, but since the outlet port is beyond the bounds of the model system, it does us no good to consider it double-ended, and we treat these by-products as lost, or sinked, instead. Note, however, that here, as elsewhere throughout the model, such losses are explicitly channeled.

The final category of system element is the processing block. In our present model, the sole example of these is the refining block. The isolated-phase view permits a refinery model in which crude oil is sinked and petroleum products and refining by-products are separately sourced. The sink-source representation emphasizes that our information regarding the refinery is isolated to an accounting of what flows into it and what it produces; pending better internal refinery information as adequate models are developed, we can still operate the remainder of the system. As in other portions of the model, this allows us to isolate potential error sites from sites at which we expect to have adequate data, and thus to control inaccuracy in the system far better than we could otherwise. For lack of a better term, we refer to refining as "hybrid" since we have modelled a conservative process with non-conservative elements.

Figure 4 shows what a portion of the Figure 1 flow model might look like when composed out of the generalized blocks that have been presented. The level of monitoring control attained by use of the restricted block interconnections is evident and is, we believe, one of the principal advantages of the present approach. For purposes of illustration, the port interconnections in Figure 4 are represented as vector queues. The connections would be direct, of course, but the intent is to demonstrate that the distinct, but lossless, event sequences at connected ports need not occur in synchrony.

APPLICATIONS OF THE MODEL

An information system predicated on the material flow structures outlined here should operate to advantage in responding to several important classes of queries. A major utility of the present approach, in this context, is the direct link between the actual physical flow relationships represented and the matrix storage structure that could reasonably be expected to constitute the eventual data repository; the closeness of this bond between conceptual formulation and data structuring greatly enhances combinatorial data manipulations of all types, including entry, validation, access, retrieval, flagging, and modification.

As has been mentioned, the model contains no forecasting or prediction capabilities; rather, it is intended as a prototype methodology for organizing information on existing situations. A useful definitional bound for forecasting, in this regard, is that of stationarity: a system such as this one can project reasonably only over an interval during which all state variables can be held stationary, i.e., over a single time step, such as, say, one month. Longer term prediction cannot be accurate if it is based merely on projection, since projection is not sensitive to cusps and discontinuities in the state variables. Within the bounds of the stationarity restriction, the data model presented here might answer questions relating to instantaneous remaining emergency capacity, but questions relating to the effects of gasoline price on consumer demand would be, by intent, out of bounds. Similarly, one would not ask this system when the U.S. will run out of crude oil, but the system would be useful, for instance, in suggesting the short term effects of an oil exportation reduction in Iran on New England.

An initial list of query classes addressable by an information system based on the model might contain the following:

(1) Aggregation: Material or dollar volume totals, or average price, cumulated by state, corporation, facility, usage, industry (e.g., utility or transportation), material, price tier, transport facility, etc., over varying time periods, in any combination (e.g., corporate by state, PAD region, etc.)--these aggregate data are either identically stored in the system or are immediately calculable from data that are stored. Other data can be either exactly calculated, approximated, or inferred from stored data: profit at each stage, cost versus profit at each stage, value added. Further, cyclical, or otherwise time dependent, information can be selectively accessed and plotted: seasonal importation, consumption, or production (aggregated over U.S., or by state, company, region, etc.), etc.

(2) Process chaining and families: Supplier/customer communities for individual facilities, regions, companies, products, etc., rank-ordered by product or dollar volume, possibly with seasonal variations. Primary path tracing and distributions for various products from source to end use.

(3) Supplies on hand and emergency preparedness: Volumes instantaneously in system, by product. Instantaneous maximum storage capabilities. Transportation staging and production lag times to respond to various perturbations (such as export cessation from Iran). Regions primarily affected and recovery response time course; re-radiated, reflected and residual effects on various parts of the system of local or focused perturbations.

(4) Verification and support data for longer range forecasting, although not the forecasting projections themselves.

(5) Information validation: Internal and external validation, cross-checking of data (e.g., monthly facility inventories compared against shipment/receipt data; shipment information from source facility compared against receiving information from destination facility). Data conditional flags and sentinels. (Validation is central to the entire data manipulation process, since the usefulness of the system is compromised unless data accuracy can be assured.)

(6) System sensitivity to policy modifications: Given an assumed or estimated consumption efficiency increment, what percentage improvement of regional or U.S. petroleum usage would be expected from a national 55 mph speed limit or from restricting government office buildings to 65°F heating?

Given a new energy extraction process (shale oil, for example) and its associated estimated yields and costs, what percentage of present consumption could it support (and in what regions and product sectors), and how close are present energy costs in these sectors to the point at which the new process becomes cost effective? (Per the discussion introductory to this section, the model addresses present situations only: (1) consumption support of the new process is estimated based on instantaneous present state data only, and is not projected forward; (2) no attempt is made to consider closed-loop effect on the market price of the energy derived, since the present model does not contain a representation for demand.)

SUMMARY

We feel we have developed a viable prototype data representation for use in highly interconnected environments such as the petroleum supply and distribution system treated here. While we do not claim rigorous completeness regarding the intricacies of the system, the overall structure, an ensemble of databases connected by explicit mathematical relations, is modular and uniform, and forms a suitable basis for predication of an information system covering this field.

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