

PLANNING OF AN INTEGRATED PETROCHEMICAL COMPLEX USING SCMART®

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Abstract. The operation of a petrochemical complex (Schulz et. al, 2003) is optimized using a new optimization tool for planning and scheduling. In the present work, an integrated site section is optimized, with nine production plants and their logistics. This consists of two ethane fractionators, two ethylene crackers, four polyethylene reactors and one chlorine vinyl monomer plant. The optimization model includes the integrated mass balance for the petrochemical pole supply chain. It is important to remark that all the plants are connected by pipeline and there are contracts with “take or pay” and “delivery or pay” clauses. This means that there are commercial obligations between them. The system has many constraints and restrictions as lack of raw material, lack of ethylene demand, lack of polyethylene demand, availability and seasonability due to lack of natural gas or raw material high prices. The resulting model is a mixed integer nonlinear programming (MINLP) problem. In this work we try to facilitate decision making/taking process for Supply Chain people, calculating variable costs for final products, and optimal ethane taking for a multiperiod problem. The problem is solved using Optience SCMart Suite (Optience Corporation). This tool uses an equation based modeling approach with state of the art optimization technology capable of solving from LPs to MINLPs. This optimization software solves the problem in the actual model formulation, without using “recursive linearization” techniques and ensures a local optimal solution.

Keywords: Supply Chain, Integrated Site, Planning, Scheduling, Petrochemical Complex

1. Introduction

Operating planning for an integrated petrochemical site is a fairly complex and challenging problem. The manufacturing process typically starts with a plant with the flexibility of processing various qualities of feedstock, which provides the raw material for downstream plants that produce different products.

Supply Chain management in the petrochemical manufacturing industry is normally being performed either as a “handmade task” using spreadsheets or with different Planning and Scheduling commercial systems. These packages usually have some lack of functionality that comes from the limitations of solution methods used and from the incapability of providing a full integration between the Planning and the Scheduling levels.

In this work we solve the supply chain planning problem of a sector of a Petrochemical Complex using a new tool: the package SCMart. This new tool uses state of the art solvers for Linear Programming and Mixed Integer Nonlinear Programming Problems.

Supply Chain people are currently faced to several planning and/or scheduling problems that must be solved every day, week, month or quarter. Some typical problems are “ethane taking optimization”, “production plan”, “export or import operations”, or “product demand satisfaction”. SCMart Suite for Planning and Scheduling is a robust tool that can solve of these types of problems and supports business decisions. It is based on an advanced optimization technology and a database centric system architecture which provides a flexible data management. Users can generate their own models under the friendly graphical interface SCMart Modeler where each unit

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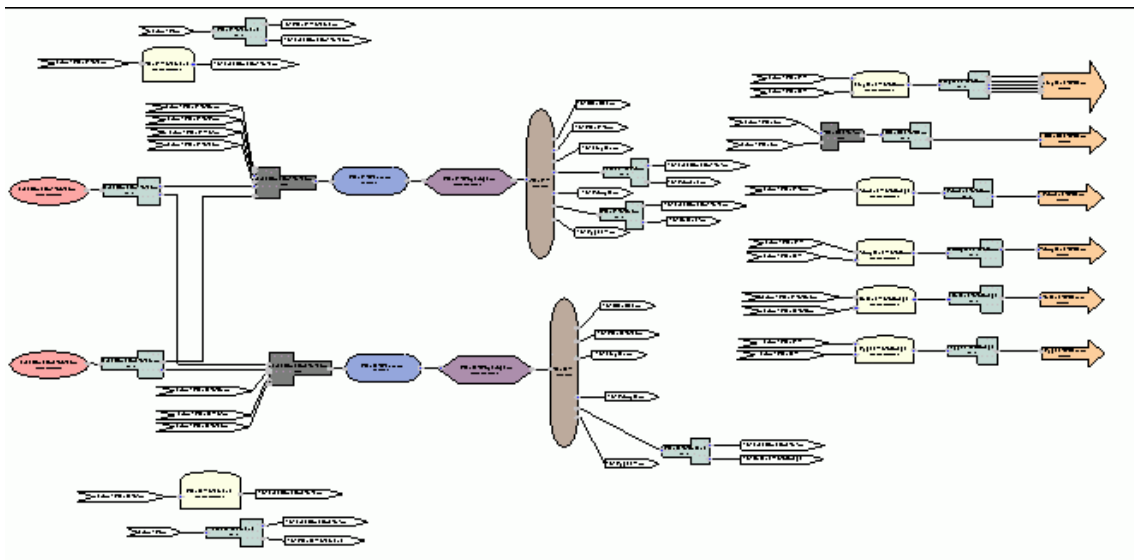
operation is represented by a task, which has its own variables and parameters. SCMart Modeler has incorporated many useful tasks as reactors, splitters, mixers, demands and suppliers.

When the model design is finished, it is possible to generate multiperiod case studies that allow the users to optimize the entire supply chain, from operation conditions to managing inventories. After running the optimization an optimal solution is reached and the results can be browsed using a flexible interface.

2. Process Description

The Fig. 1 describes the flowsheet as implemented in SCMart. It consists of a Petrochemical Complex with two ethane fractionators, two ethylene plants and five ethylene consumers. Each fractionator is connected through a pipeline to both ethylene plants, and then they can feed one or both of them simultaneously. Two ethane storage tanks are available to cover lack of raw material from the fractionators along the year.

Fig. 1: Flowsheet of an integrated petrochemical complex



The ethylene plants consist of ethane cracking and acetylene reactors, and a cold product separation area that provides ethane, propane, propylene and butane recycles to the crackers. In the cold section there are separation towers from which the ethylene is obtained. Other products are propane, one by plant in order to separate the main products: ethylene with a 20000 tons storage tank and byproduct streams like propane, propylene, butane and pygas. Besides non-converted ethane returns to the furnaces and rich gas is used as raw material in the utilities area.

Finally, the flowsheet of Fig. 1 has a separation section, which produces the different products for the five ethylene demands (polyethylene plants), and the four by-product demands (propane, propylene, butane, and pygas). Part of the propane, butane and propylene are recycled to the furnaces.

3. User and Model Interfaces

In this section we make a quick description of the User and Model interfaces of the package SCMart.

3.1 The user interface:

SCMart has a friendly user interface to interact with the Core files. These files do not belong to the Models, they are only a set of views and actions that allow the user to manipulate the model.

The Optience Core Platform is the engine needed to open the SCMart Suite Core Files. An online help provides an explanation of the menus and commands that are available on launching a Core Application. These commands are common to any application built using the Core Framework and therefore apply to any SCMart Models.

3.2 The model interface:

The Model Interface is implemented as a set of four Views with their corresponding Nodes. The Views are: i. Model Manager; ii. Case Manager; iii. Case Definition; iv. Case Results.

- i. **Model Manager:** The Modeler Manager View is the starting point for browsing and creating models in SCMart. This view displays the list of available Models. In this view you may complete all data in the Master Information node, which have five sub-nodes: Material Sets, Materials, Plants, Model Types and Color. Models Node allows the user create new models and search for a desired model which has been created previously. SCMart Modeler is the graphical interface for modeling in SCMart Suite. Each unit operation is represented with a task and each task has its own variables and parameters. Only the material balance is modeled, but not only material based variables are considered. Other variables and properties that affect the mass balance can be included (COT, SG, etc). Finally in the Solver Options Node the user can find different model types (MILP, MINLP, NLP and RNLP) and set their parameters in the *Value* column for each field option (i.e. iteration limit).
- ii. **Case Manager:** In the Case Manager View the user can generate, copy, paste and delete Cases. Also data information can be transferred from different models. In order to develop sensitive analysis, subcases could be generated in this node. Once the model is created (with all tasks, streams and related equations), a new case must be created in order to run the model. A case is a particular situation of plant operation. It could be interesting to run the case in the design capacity, normal operation or maximum capacity modes, setting the number of daily or monthly periods. Model Name Node allows to create different cases. In this node, two grids are displayed in the Node Window: Model and Cases grids. Case Name Node displays all the information about the current case and it is the point where subcases or sensitive analysis can be created. Subcases can be generated to see the effect of a given parameter, coefficient or variable bounds on the optimal solution of the problem.
- iii. **Case Definition:** In the Case Definition View the different cases and subcases previously created lower (Min) and upper (Max) variable and parameters values per period. The chemical reactions and equations coefficients can also be changed. The information required to define a case is problem dependent but it can be classified according to its type. Each view for entering information can consist

of one or more grids, which may contain the same or different type of information. The user can define following items:

- *Parameters Grids*: Values of Parameters of a case and/or their subCases. These kind of grids allow the entering of prices, production costs, separation ratios, yield coefficients and all other parameters that do not depend on the time period.
 - *Parameters PD Grids*: Values of Period Dependent Parameters of a case and/or their subCases. Here you can also define prices, production costs, separation ratios, yield coefficients and all other parameters, but in these cases they are period dependent. These views always include the period column.
 - *Variables Grids*: Maximum and minimum values of Variables of a case and/or their subCases. These grids always include the *Min* and *Max* column for entering the limits of the variables for each period. They might also contain the *Value* column, in these cases this value is used as initial point for the optimization. The only way to fix a variable is making $Min = Max$.
 - *Binaries Grids*: Maximum and minimum values of Binary variables of a case and their subCases. Here, can also be also found the *Min* and *Max* columns which can only be zero or one. The grids might also contain the *Value* column that can also take the values zero or one, this value will be used as initial point during the optimization phase to start looking for an integer solution.
 - *Ranges Grids*: Maximum and minimum values of Ranges of a case and their subCases. For these grids the *FromPeriod* and *ToPeriod* columns are shown to indicate the range of the variable. As in other cases, the *Min* and *Max* columns can be edited and the *Value* column might be present.
 - *Equation Coefficients Grids*: Values of Equation Coefficients of a case and/or their subCases. These values can be for yield reactors, custom separations or user equation tasks. The coefficient values can be period dependent or not, depending whether the *Period* column is shown or not.
 - *Conversion Coefficients Grids*: Values of Reaction Coefficient of a case and their subCases. These grids display the *Value* of the conversion reactors coefficients. They can be period dependent or not, depending whether the *Period* column is shown or not.
- iv. Case Results: In the Case Results View model cases are optimized and the results obtained are checked. In the *Optimize@Client* Node, the models will be optimized. Every time the users are interested in checking the current SOLVER run, they can "save" it. In the *Solution* Node, the optimization results can be checked. Clicking on this node a grid is shown. It is composed of *SubCase ID*, *Subcase*, *Solution*, *Item*, *Value* and *Comment*. For each subCase three items are displayed: *Solution Status*, *Total Model Infeasibility* and *Objective Function Value*. The results appear as children nodes in grids and graphs. The type of information that can be found in this node is as follow: Finance (profit, shadow prices, costs), Supplies, Demands, Inventories (raw materials, intermediates, products), Production, Balances, Physical Limits

4. Model Description

We developed a case of study for a 12 months horizon with non-period dependent parameters (as raw material or inventory costs) and period dependent parameters (as product demand prices and flows), and raw material availability.

Overall and components mass balances (Hydrogen, Methane, Ethane, Acetylene, Ethylene, Propane, Propylene, Butene, Butane, Pentane, Water) were performed. Constant split factors were used to simulate the towers. The two ethane suppliers produce about 52 ton/h and 71 ton/h respectively.

Figure 2 shows how yield reactor are modeled in SCMart. Several predefined or custom equations types can be used.

Fig. 2: Linear Furnaces Equation types

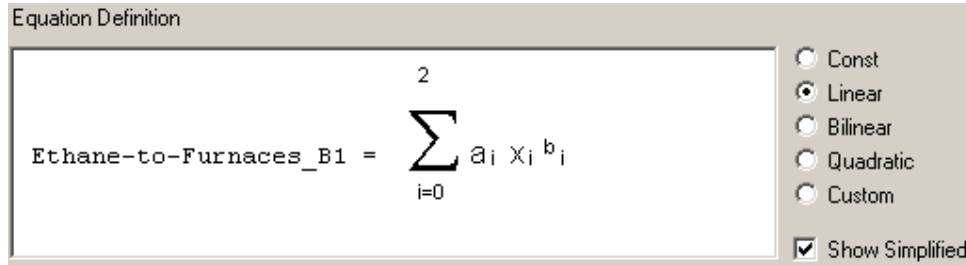


Figure 3 shows how conversion reactors are modeled.

Fig. 3: Acetylene Reactors Equations

	Stream	Material	Value
▶	CrackedGas-to...	ACETYLENE	-1
	CrackedGas-to-Hy...	H2	-0.077
	HydrogenatedGas...	ETHYLENE	1.077
*			

Tables 1, 2, 3 and 4 show SCMart Case Definition Views for the complete set of input data of the case studied presented in this paper. Data are raw material availability, product demand and product prices profiles along the year.

Table 1. Ethane Fractionator 1 (Raw Material Availability)

	SubCase	Period	Stream	Variable	Min	Value	Max
	Stream : Ethane-to-split						
	Base	2005-03	Ethane-to-split	flow	14.4	30	30
	Base	2005-04	Ethane-to-split	flow	14.4	33	33
	Base	2005-05	Ethane-to-split	flow	14.4	33	33
	Base	2005-06	Ethane-to-split	flow	14.4	27	27
	Base	2005-07	Ethane-to-split	flow	14.4	27	27
	Base	2005-08	Ethane-to-split	flow	14.4	27	27
	Base	2005-09	Ethane-to-split	flow	14.4	37.5	37.5
	Base	2005-10	Ethane-to-split	flow	14.4	37.5	37.5
	Base	2005-11	Ethane-to-split	flow	14.4	37.5	37.5
	Base	2005-12	Ethane-to-split	flow	14.4	33	33
	Base	2006-01	Ethane-to-split	flow	14.4	33	33
	Base	2006-02	Ethane-to-split	flow	14.4	30	30

Table 2. Ethane Fractionators 2 (Raw Material Availability)

	SubCase	Period	Stream	Variable	Min	Value	Max
	Base	2005-03	Ethane-to-split	flow	21.6	45	45
	Base	2005-04	Ethane-to-split	flow	21.6	45	45
	Base	2005-05	Ethane-to-split	flow	21.6	45	45
	Base	2005-06	Ethane-to-split	flow	21.6	51	51
	Base	2005-07	Ethane-to-split	flow	21.6	51	51
	Base	2005-08	Ethane-to-split	flow	21.6	51	51
	Base	2005-09	Ethane-to-split	flow	21.6	48	48
	Base	2005-10	Ethane-to-split	flow	21.6	48	48
	Base	2005-11	Ethane-to-split	flow	21.6	45	45
	Base	2005-12	Ethane-to-split	flow	21.6	42	42
	Base	2006-01	Ethane-to-split	flow	21.6	42	42
	Base	2006-02	Ethane-to-split	flow	21.6	42	42

Table 3. Polyethylene Reactors (Ethylene Demand Seasonability)

Period : 2005-04						
Base	2005-04	Ethylene-to-PE1	flow	6.48	7.5	7.5
Base	2005-04	Ethylene-to-PE2	flow	6.48	7.5	7.5
Base	2005-04	Ethylene-to-PE3	flow	7.2	9	9
Base	2005-04	Ethylene-to-PE4	flow	14.4	22.5	22.5
Base	2005-04	Ethylene-to-VCM	flow	7.2	9	9
Period : 2005-05						
Base	2005-05	Ethylene-to-PE1	flow	6.48	7.5	7.5
Base	2005-05	Ethylene-to-PE2	flow	6.48	7.5	7.5
Base	2005-05	Ethylene-to-PE3	flow	7.2	9	9
Base	2005-05	Ethylene-to-PE4	flow	14.4	22.5	22.5
Base	2005-05	Ethylene-to-VCM	flow	7.2	9	9
Period : 2005-06						
Base	2005-06	Ethylene-to-PE1	flow	6.48	8.1	8.1
Base	2005-06	Ethylene-to-PE2	flow	6.48	8.1	8.1
Base	2005-06	Ethylene-to-PE3	flow	7.2	9.6	9.6
Base	2005-06	Ethylene-to-PE4	flow	14.4	23.1	23.1
Base	2005-06	Ethylene-to-VCM	flow	7.2	9.6	9.6

Table 4. Polyethylene Reactors (Ethylene Prices Seasonability)

Period : 2005-04				
Base	2005-04	Ethylene-to-PE1	flwVal	350000
Base	2005-04	Ethylene-to-PE2	flwVal	350000
Base	2005-04	Ethylene-to-PE3	flwVal	330000
Base	2005-04	Ethylene-to-PE4	flwVal	320000
Base	2005-04	Ethylene-to-VCM	flwVal	330000
Period : 2005-05				
Base	2005-05	Ethylene-to-PE1	flwVal	350000
Base	2005-05	Ethylene-to-PE2	flwVal	350000
Base	2005-05	Ethylene-to-PE3	flwVal	330000
Base	2005-05	Ethylene-to-PE4	flwVal	320000
Base	2005-05	Ethylene-to-VCM	flwVal	330000
Period : 2005-06				
Base	2005-06	Ethylene-to-PE1	flwVal	420000
Base	2005-06	Ethylene-to-PE2	flwVal	420000
Base	2005-06	Ethylene-to-PE3	flwVal	396000
Base	2005-06	Ethylene-to-PE4	flwVal	384000
Base	2005-06	Ethylene-to-VCM	flwVal	396000

5. Results

After running the SCMart optimization case, results can be visualized through a set of tables. Table 5 is a first table presenting the optimum value of the objective function and the status of the run. In the application example presented in this paper, the total profit for the flowsheet of Fig. 1 was $62.0 \cdot 10^6$ US\$/year or $5.2 \cdot 10^6$ US\$/month. The profit is calculated as $\text{PROFIT} = \text{FLOW VALUE} - \text{FLOW COST} - \text{INVENTORY COST}$

Table 5. Optimization Run

Solution					
Drag a column header here to group by that column					
	SubCase	Solution	Item	Value	Comment
▶	Base	1	Solution Status	1	Optimization was Successful
	Base	1	Total Model Infeasibility	0	
	Base	1	Objective Function Value	62.5521	

Table 6 shows a desegregation of optimal values for main economic variables as profit, product value (flow value), raw material cost (flow cost) and inventory cost.

Table 6. Optimization Results

	SubCase	Solution	Description	Value
▶	Base	1	Profit	6.25521E+07
	Base	1	Flow Value	3.147417E+08
	Base	1	Inventory Value	0
	Base	1	Flow Cost	-2.521243E+08
	Base	1	Inventory Cost	-65314.26
	Base	1	Product Inventory Cost	0
	Base	1	Production Cost	0
	Base	1	Transportation Cost	0
	Base	1	Product flow Value	0
	Base	1	Product Inventory Value	0
	Base	1	Product Flow Cost	0
	Base	1	Product Production Cost	0
	Base	1	Product Transportation Cost	0

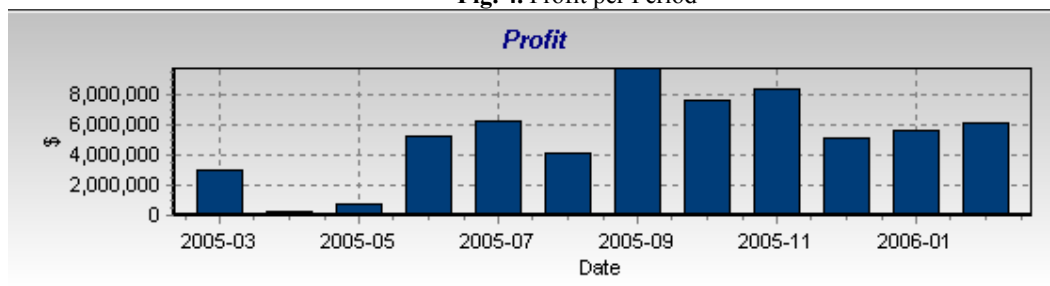
Table 7 shows the optimal profit profile along the time horizon.

Table 7. Profit per Period

SubCase	Period	Value
► Base	2005-03	2972238
Base	2005-04	213166.5
Base	2005-05	754323.9
Base	2005-06	5255147
Base	2005-07	6340590
Base	2005-08	4186033
Base	2005-09	9817496
Base	2005-10	7657496
Base	2005-11	8428783
Base	2005-12	5140206
Base	2006-01	5650590
Base	2006-02	6136033

Fig. 4 shows the same profit result in bar graphic. During the first three months, little benefits are obtained and while they increase along the rest of the year due to product prices seasonability. In the first periods low product prices motivate a little Profit. After month 3, product prices are higher while the raw material keep constant generating a larger profit.

Fig. 4. Profit per Period



In Fig. 5 we observe the profile for the income from ethylene selling. A similar behavior as for the profit can be observed during the first three months. In the rest of the year flow value increases due to a higher demand and prices. The maximum product value is reached at periods 9, 10 and 11.

Fig. 5. Flow Value per Period

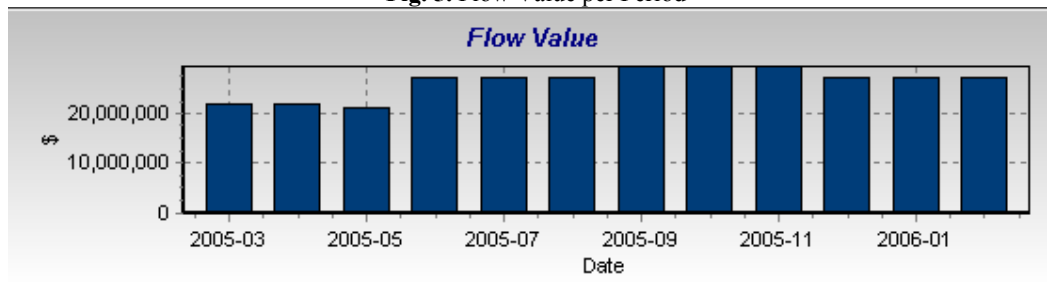


Fig. 6 shows the cost value profile. As can be observed it is quite stable due to raw material fixed costs. The variation observed comes from the raw material availability profile. In period 8 and 12, the larger value cost are reached due to the higher raw material availability and demands during these periods.

Fig. 6. Flow Cost per Period

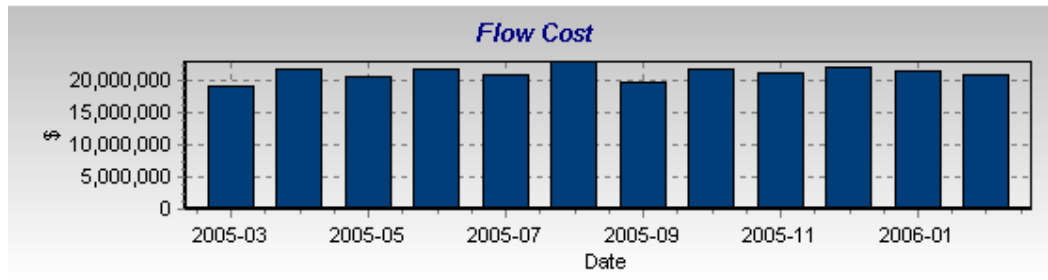
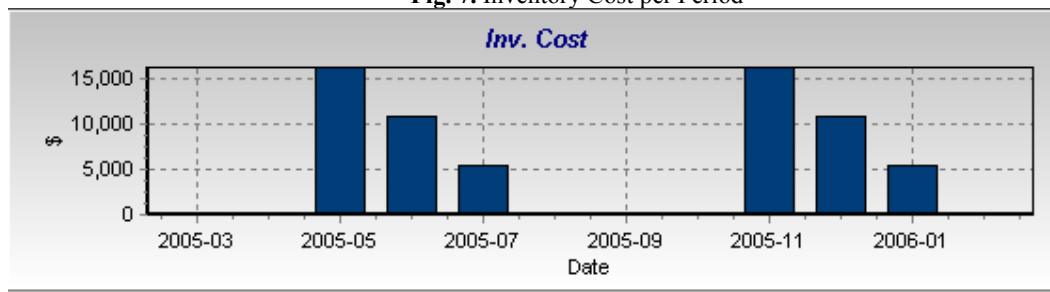


Fig. 7 shows inventory cost profile. It increases during the periods 5 up to period 7, and from period 9 up to 11, because larger raw material availability and lower product demands during these periods.

Fig. 7. Inventory Cost per Period



5. Conclusions

In this paper we have described a new tool (SCMart) for planning and scheduling problems, with application in Petrochemical and Refinery Plants. This software is a user friendly and fast environment for solving large planning and scheduling optimization problems. It has easier to use sensitive analysis capabilities, allowing the user to change any different optimization parameters to study its impact on any calculated variable. In this paper we have presented the computational tools and application results corresponding to a typical planning problem in a petrochemical site consisting in the integrated operation of several plants. Considering that the package naturally integrate operational and commercial aspects, it is also a useful tool for business planning.

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