





Chapter 8

Conclusions

This thesis presents the different parts of a global generic framework for planning and scheduling of batch chemical plants. Different components have been studied: a data model, a timing model, sequencing and assignment strategies and optimization.

The data model presented in this thesis allows an organized and systematic information management dealing with the detailed representation of batch processes in the chemical industry. It allows the representation of:

- Recipes with an unlimited number of stages and operations.
- Time relationships between operations.
- Complex storage constraints
- Unit constraints.
- Material constraints.
- Calendar availability.
- Demand requirements.

The model is also extensible as it is object-oriented and allows the inclusion of new properties in all the objects defined. This model is flexible enough to be used with very different scheduling techniques.

The EON model for operations timing is one of the main contributions of this thesis. The main strength of the EON model is the capability of representation of complex time constraints between operations in the same schedule using simple components as events, operations and links.

The construction of the EON for different kinds of links has been discussed as well as a methodology for the representation of storage constraints as time constraints. The treatment of storage constraints as time constraints represents also a new approach to the complex storage constraints present in the chemical industry. An iterative procedure also allows taking into account of limited resources.







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Two different methods for calculating the EON model have been shown and compared. The FCEON method based on a iterative procedure has proven to be faster than the formal LP formulation for solving EON models. Nevertheless, both approaches have proven to be fast enough to deal with models up to 7000 operations with less than 8 seconds of CPU time. This fact shows that both methods are suitable to deal with complex chemical problems.

Regarding the sequencing assignment and online scheduling, dispatching-like rules have been used for the calculation of the material balance, the unit assignment and the batch sequencing. The strength of this approach is based in the easy implementation and adaptation to a batch oriented framework. Additionally, the application of these rules can end up with optimal or near optimal schedules. These rules can be applied to empty schedules or to schedules that already contain *frozen* batches, which represents the actual situation in the plant. This last aspect allows the use of this kind of rules when performing on-line scheduling.

Different optimization techniques have been used in this thesis to solve the scheduling approach presented. Stochastic and mathematical methods has been used and tested.

Regarding to the stochastic methods, a new optimization algorithm (MSES) has been introduced that improves the performance of the SA standard algorithm. A modified GA algorithm has also been proposed that transforms the infeasible sequences commonly generated into feasible ones. All the stochastic methods used were adapted to batch processing structures involving batch sequencing and rule driven unit assignment.

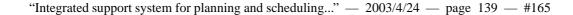
Regarding to the mathematical approach, the mathematical formulation presented in then EON timing model has been extended by introducing sequence and assignment variables as well as storage constraints.

A motivating example has been taken as a test case. All the optimization approaches presented as well as all the sequencing algorithms have been executed in the test case and the results compared. The GA approach has been shown as the best approach for this case study, finding the best solution in most of the scenarios used.

Despite of the good performance showed by the GA in the case study presented, one cannot conclude that the GA implementation used will be the best in all cases. SA and MSES are easier to implement than GA and also provide good results. Otherwise is important to note that a simple combination of sequencing rules can also find the best solution in more than 50 % of the scenarios tested. The MILP formulation presented can assure the mathematical optimum. Actual improvement of computer processors and solvers used to solve MILP formulations has permitted to solve bigger and more complex problems in less CPU time. However, comparative tests cases realized show that most of industrial-size problems still require other approaches than MILP rigorous solutions because of prohibitive computation times.

One of the strongest points of the framework presented is its modularity. The fact of having the different components of planning and scheduling as separate modules sharing a common data model allows and easy use and adaptation of different techniques that can help solving the scheduling and planning problem in specific cases. This modular approach has been useful when applying the techniques presented to industrial scenarios. Adaptation to specific scenarios choosing the best alternative for each one is possible and easy. The key point for achieving this is to share the common data and timing model (the EON model). Additionally, the use of a data model based in the ISA S88 standard allows also the integration of the scheduling and planning with the control level. This on-line integration has been

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successfully achieved using a pilot plant scenario.

Summarizing the conclusions, the main contributions of this thesis are:

- Developing of a common data model compatible with the ISA S88 standard.
- Creation of a new timing and temporal constraint representation model (EON) capable to handle complex temporal constraints, including storage and resource constraints.
- Assessment of different sequencing and assignment procedures within the data and timing model created
- Development of a new optimization procedure (MSES) and a new MILP model (EONX) for the scheduling of batch chemical plants.
- Adaptation of other optimization techniques (SA and GA) to the data and timing model presented.

Future work

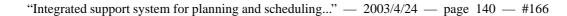
The work presented in this thesis can be taken as a basis for future enhancements. In this sense several P.h.D. Thesis are currently undergoing underway in the following topics.

- Improved rescheduling methodologies: This thesis has only developed the basic framework for on-line scheduling. Further improvements are needed in order to find the best methods and rules to be used within an on-line rescheduling environment.
- Optimization under uncertainty: This thesis only deals with deterministic times and demand. Further work is necessary to include in he present work methodologies that allows the incorporation of the uncertainty in the planning and scheduling procedures.
- Multi-objective optimization: The optimization methods presented in this thesis only
 deal with a simple objective function. Multi-objective optimization is necessary to
 include more than one objective function in the evaluation of the different scheduling
 alternatives.
- Interaction with upper decision levels: The integration of the production scheduling level within a supply chain level can help to find the optimum management for the entire supply chain.
- Incorporation of forecasting techniques: Forecasting can be use either to calculate future demands as well as to calculate the evolution of the future operation times and maintenance tasks (i.e. evaluating the TOP of operations with decaying performance).

Other future works that can be taken into account are:

Distributed optimization: the use of distributed computing can allow the exploration
of a bigger solution space. Optimization techniques such as memetic algorithms and
distributed GA are out of the scope of this thesis but can be easily introduced in the
framework presented. A distributed client-server or agent based optimization approach









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could be interesting as a solution for finding the optimal solutions for industrial scenarios. The distributed approach can also be useful when dealing with multi-objective optimization.

• Scheduling and simulation: The incorporation of first principles simulation models in the scheduling framework can help the determination of more accurate process times taking into account characteristics as the quality of the raw material or the effect of changing the setpoints of the process.









B: Set of batches.

 BS_b : Batch size of batch b.

 C_i : Charge (level increase) of an storage.

 D_i : Discharge (level decrease) of an storage.

 DN_k : Destination event of link k.

MAX: Maximum level associated to an storage.

MIN: Minimum level associated to an storage.

 μ_n : Discharge index associated to charge n.

 K_n : Fraction of discharge μ_n .

 v_m : Charge index associated to discharge m

 κ_m : Fraction of charge υ_m

 C_i : Charge (level increase) of an storage

 D_i : Discharge (level decrease) of an storage

 DN_k : Destination event of link k

 EE_{mb} : End event associated to F_{mb} .

ET': Finishing time of operation'









 ET_n : Finishing time of operation n.

 EN_{bs} : End event associated to the stage s of batch b.

 F_{mph} : Flow associated to the material m of the batch b that is assigned to the storage g.

 F_{mb} : Flow of material m of the batch b.

 FN_m : Final event of operation m.

 FN_m : Final event of operation m.

 G_m : Set of storages storages associated to the material m.

 IN_m : Initial event of operation m.

 I_m : Initial stock level of material m.

 I_{S} : Initial level associated to storage S.

 $I_{S,m}$: Initial level associated to storage S and material m.

IT': Starting time of operation'.

 IT_n : Starting time of operation n.

K: Delta time.

 K_n : Fraction of discharge μ_n .

MAX: Maximum level associated to an storage.

 MAX_m : Maximum storage capacity for material m.

 MAX_S : Maximum storage capacity for storage S.

MaxUnits_{bs}: Maximum number of units that can perform simultaneously the stage s of batch

 Max_{mg} : Maximum level for material m in storage g.

 Min_{mg} : Minimum level for material m in storage g.

MIN: Minimum level associated to an storage.

 MIN_m : Minimum storage capacity for material m.

 MIN_S : Minimum storage capacity for storage S.

MS: Makespan value.

 $N_m(SC)$: number of level variations of material m in the partial schedule.

 $N_s(SC)$: Number of level variations associated to storage s .









 NI_{V_n} : Initial event of variation V_n .

 NF_{V_n} : End event of variation V_n .

 ON_k : Origin event of link k.

P: Probability.

 $P_{bb'}$: Binary variable which relates a pair of batches (b and b'). If batch b is processed before batch b' then the predecessor variable $P_{bb'}$ equals to 1.

 Q_u : Capacity of unit u.

 S_b : Set of stages of batch b.

SC: Partial schedule.

 SE_{mb} : Start event associated to F_{mb} .

 SF_{bsu} : Size factor associated to the batch b, the stage s and the unit u.

 SN_{bs} : Start event associated to the stage s of batch b.

 TOP_n : Operation time associated to the operation n

 TW_m : waiting time of operation m

 TW_m^{max} : Maximum waiting time for operation m

 $TWmax_n$: Maximum waiting time for the operation n

 T_n : Time value associated to event n

 T_n^{min} : Minimum time associated to event n

U: Set of units.

 U_{bs} : Set of units that can perform the stage s of batch b.

 V_i : Level variation of an storage.

 $V_{m,i}$: Level variations for material m.

 $V_{S,i}$: Level variations for storage S.

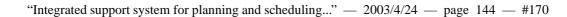
 X_{mbg} : Binary variable which is 1 then the flow of material m of the batch b (F_{mb}) is associated to the storage g.

 Y_{bsu} : Binary variable which equals to 1 if stage s of the batch b is allocated to unit u.

Z: Objective function value.

 ΔT_k : Delta time associated to link k.









 $\Delta(OF)$: Change in the objective function.

 $\alpha_{S,i,m}$: Binary variable equal to 1 if the variation $V_{S,i}$ refers to material m.

 κ_m : Fraction of charge v_m .

 Ω_0 : Solution space of n! possible sequences.

 ω_i : Sub-space $\in \Omega_0$.

 μ_n : Discharge index associated to charge n.

 υ_m : Charge index associated to discharge m.









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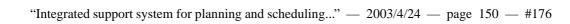




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Appendix A

MOPP: A generic scheduling package

A.1 Background

MOPP is the name given to the different versions of the scheduling package developed in the Chemical Engineering Department of the Universitat Politecnica de Catalunya during the last 20 years of research in this area.

The first implementation of MOPP was developed on a VAX-VMS computer system and it was programmed using FORTRAN language. The input were raw text files whilst the output were also text files and printed gantt-charts (see figure A.1).

The availability of new computer power in the form of Unix workstations allowed the development of new versions during the lasts 80's and the first half of the 90's. These versions of MOPP had an improved graphical user interface (programmed in C), an electronic gantt-chart and improved algorithms including support for resource constraints and optimization using simulated annealing (see figure A.2). Most of the input data were provider either via raw text files or via relational databases (depending on the problem size). The UNIX versions of MOPP were successfully applied to industrial cases as big as Punto Blanco (a socks factory) with 20.000 different production recipes with the corresponding changeovers and additional constraints.

The main drawback of these versions was the use of a fixed task structure composed by 5 operations that could be active or not (preparation, charge, operation, discharge, cleaning). This aspect was a strong drawback when more complex recipe structures were required.

That was the scenario when this thesis begun. At the beginning of this work two main objectives for the next versions of MOPP were defined:

- Creation of new models for the timing and recipe description that could handle complex recipe structures
- Creation of a new version of MOPP running on windows NT instead of UNIX as the









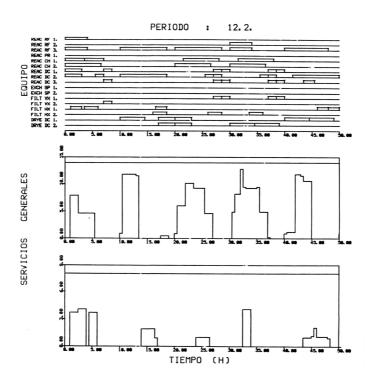


Figure A.1: Output of the first version of MOPP (1985)

industrial partners were also switching from UNIX to Windows NT.

During the last 90's until 2000 a new version of MOPP was developed running under windows NT which has the following characteristics:

- The development was carried out using C++Builder under Windows NT.
- It had a complete user interface for input and examine all the data involved.
- The EON model was developed and introduced in the system as a way to describe complex time constraints within the recipes
- A flexible recipe structure based on 3 description levels (process-stage-operation) was introduced. The concept of links between operations was also developed and tested.
- An object-oriented data structure was used, allowing customizations by switching one object by another.









A.1. Background

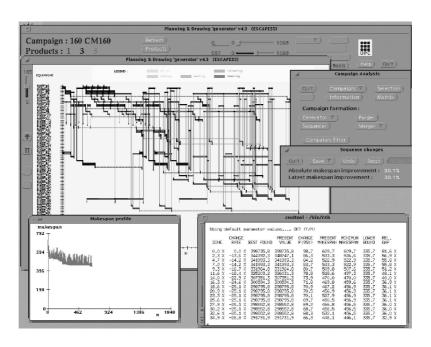


Figure A.2: Screenshot of a UNIX MOPP version(1995)

- An improved electronic gantt-chart was developed.
- It handles resource constraints.
- It handles time constraints such as unit unavailability from an specific time to another.
- It provides two different standard optimization algorithms such as SA and MSES.

This version of MOPP was applied to different industrial cases and completely customized to be used in a ABS polymer plant. That specific version (see figure A.3) deals with more than 2000 different recipes, producing optimum detailed schedules for a 15 day periods. The input provided by files generated by SAP system allows the rescheduling of the whole plant once a day, introducing rush orders, actual state of the plant, actual storage levels and units unavailability. The plant was producing 24 hours/day, so no calendar constraints were supported.

At this point MOPP demonstrated that could handle effectively industrial-size problems and also provided a framework to allows the development of further research in the scheduling problem. Unfortunately, the design of MOPP as a monolithic application makes difficult to modify and test further enhancements. Therefore, a completely revised design was started. The new MOPP (MOPP-XXI) had to be much more flexible allowing and easy customization providing a flexible framework to allow the incorporation of new technologies and calculating procedures.



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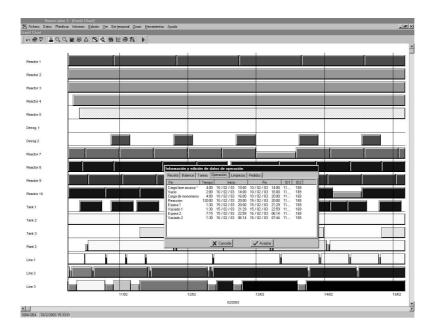


Figure A.3: Screenshot MOPP-NT customized to be used in a ABS plant

A.2 MOPP nowadays

The actual version of MOPP incorporates all the research work done in this PhD Thesis. The actual design is completely modular and plug-in-based. This design allows the incorporation of additional features and the complete customization for any specific case.

A.2.1 Key features

MOPP was designed as an aid tool for solving the scheduling problem. The actual version has the following features.

- Completely modular design
- Data model based in the ISA S88 standard from recipe to operation level of detail. It can handle:
 - Complex recipe structures and time constraints between operations.
 - Resource and time constraints depending on the processing unit used.
 - Complex storage constraints.
 - Calendar constraints
- Standard set of sequencing and assignment algorithms.







A.2. MOPP nowadays

- Different optimization algorithms (simulated anealining, genetic algorithms and mixed stochastic enumerative search)
- Open framework for the development of new plug-ins.
- Electronic gantt chart allowing direct manipulation of the schedule allowing:
 - Addition or deletion of batches
 - Changes in the assignment and sequence
 - Obtaining information
 - Modification of the constraints associated to the schedule
 - Reporting
- Configuration of objective functions

A.2.2 Structure

MOPP is designed as and open environment which allows the connection between different modules (plug-ins) which collaborate in order to perform all the tasks needed in a scheduling package. The basic idea of the MOPP structure is given in figure A.4.

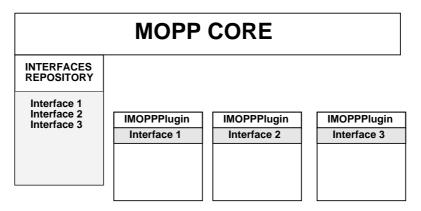


Figure A.4: MOPP structure

The MOPP core has only an interfaces repository and deals only with the plug-in management. The different plug-ins available can be loaded into the system using a plug-in manager (figure A.5) which takes care of the dependencies between the different plug-ins connected.

Each plug-in is characterized by the exposed and required interfaces. Once loaded, the exposed interfaces of each plug-in are registered in the *interface repository*. The repository is accessible by all the plug-ins, allowing the communication between them. Some of the plug-ins (those which exposes the interface IMoppGUI) are able to add new entries in the main menu. These menu entries are linked to the *run* method of these plug-ins. The execution







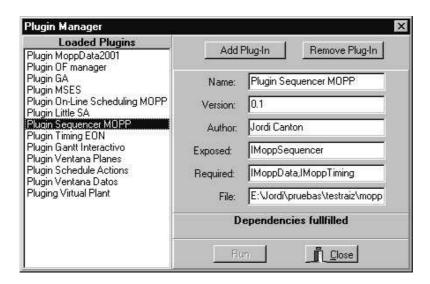


Figure A.5: MOPP plug-in manager

of the *run* method generates the sequence of actions shown in figure A.6. Usually the plugins are not designed to work alone, thus access to the other plugins trough the references contained in the *interface repository* is required to make possible that several plugins work together.

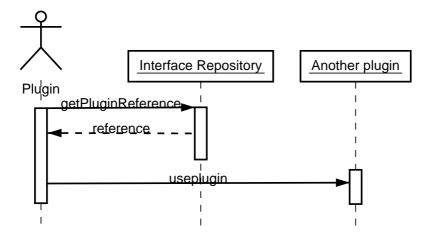


Figure A.6: Sequence diagram of plug-ins interaction





A.2. MOPP nowadays

A.2.3 Modules

The different functionalities available in MOPP are contained in a set of modules. The main modules are shown in figure A.7. These main modules are:

Data: It manages the data structure of all the data related to MOPP. This data structure is based in the model presented in chapter 3 (page 19). It also manages the persistence of the data in two ways, as XML files and as a relational SQL database.

Timing & Modeling: This is one of the main modules of MOPP, it implements the automatic building and solving of the EON structure from a given Schedule data model. It implements all the features shown in chapter 4 (page 39).

Sequencing: This module is the responsible for generating sequences of batches from an actual state of the plant and a given number of demands. It implements all the sequencing, material balance and assignment methods shown in chapter 5 (page 75).

Optimizer: There are four modules of this kind. Three of them implement the stochastic optimization algorithms (SA, MSES and GA) shown in chapter 6 (page 93). The other one generates the MILP model presented in the same chapter and solves it using GAMS.

OF Evaluation: This model allows the generation and evaluation of different objective functions. Completely new objective functions could be generated programming a new plug-in and adding it into the system.

GUI: There are several modules which offer graphical user interfaces. These modules allow the interaction with all the data and calculation modules available in MOPP. New user interfaces can be plugged into the system to generate a complete customized solution for a given industrial case.

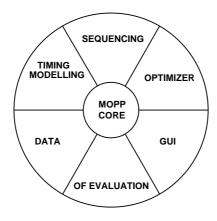


Figure A.7: MOPP main modules









There are additional modules which provide MOPP with additional functionality. These modules are:

EGC (**Electronic gantt-chart**): This module provides MOPP with a fully interactive electronic gantt chart. The user can drag & drop the different operations changing directly the sequence and the assignment of a given schedule.

Schedule actions: This plug-in provides several basic functionalities (add new batch, move batch, change assignment, etc) which allow the EGC to provide different functions applicable to the schedule.

With all the modules described, MOPP is nowadays a powerful and flexible tool capable to deal with the most complex industrial scenarios and also capable to accept further improvements with little effort. The aspect of MOPP (see figure A.8) can easily be changed developing further GUI modules suited to specific cases. Additionally, all the objects present in the data structure have a set of configurable parameters, providing an effective way to add new characteristics to any object present in the program.

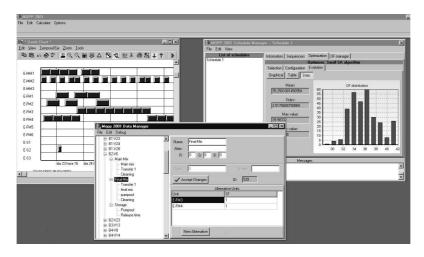


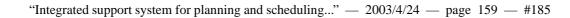
Figure A.8: MOPP XXI with several GUI modules opened

A.3 Conclusions

MOPP is currently a power and flexible package capable to deal with the complex industrial cases present in the industry. Its highly modular design makes it also valuable as a research tool in the field of the scheduling and planning problem as it can easily be used for completely different approaches. This aspects makes it valuable for comparing different solutions of the same problem using exactly the same data model as an input.











A.3. Conclusions

The structure of MOPP makes also possible to use it in specific production environments as it can support fully customized user interface and calculation modules in order to incorporate all the know-how of the specific industrial scenario.













