DYNAMIC SIMULATION OF PARTIAL DIFFERENTIAL ALGEBRAIC SYSTEMS : Application to some Chemical Engineering problems

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ABSTRACT

This contribution is devoted to the dynamic simulation of distributed models, i.e models described by a resulting set of Partial Differential Algebraic Equations (PDAE) which are commonly encountered in Chemical Engineering applications such as catalytic reactors, absorption columns,...

Here the goal of this paper is an attempt to present effective realisations , already done in different research projects in order to give experiments in this field which is very complex.

After a brief overview of classes for numerical techniques applied for Partial Differential Equations (PDE), the pros and cons on a theoretical point of view are investigated. Some of these techniques, one based on method of lines and difference schemes, and others using functional approximation method (collocation method) are presented. These methods are investigated in the general framework of Dynamic Process Simulation. It means robust dynamic simulation based on high fidelity models for realistic operational environment. Two illustrations are proposed in order to give an « air of reality » : one devoted to environmental considerations applied to wastewater treatment plants based on the use of biofilters, an other one devoted to the dynamic simulation of an absorption process

KEYWORDS : Dynamic Simulation and Modelling, Partial Differential Algebraic Equations (PDAE), Finite Difference Method, Functional Approximation Method, Biofilter, Absorption

1. INTRODUCTION : AN OVERVIEW

Dynamic simulation plays an important role in analysing and predicting the time transient behaviour of chemical and biochemical processes and is therefore very used, especially in the last decade. But , as mentioned long time ago by Heydweiller and al. (1977) and confirmed more recently by the interesting work of Oh (1995), most existing dynamic modelling and simulation tools are primarily suited to lumped parameter systems. In fact, in the reality, a large number of unit operations in Chemical Engineering such as catalytic reactors, absorption column, extraction column based on mass transfer approach and in biochemical Engineering are intrinsically distributed in nature. It means that their properties exhibit spatial as well as temporal variations. The resulting set of equations for these types of models may be viewed as a combination of lumped and distributed parameter systems, namely described by Partial Differential Equations (PDAE) submitted to initial conditions and boundary conditions.

First of all, an acknowledgement of failure has to be honestly done. Partial Differential equations (PDE) and, by the way, PDAEs arise in an enormous number of modelling applications. They are difficult to solve because change in a parameter or one of the boundary condition may lead to completely different behaviour. So, although numerical methods are suitable to solve accurately a given PDE system, other numerical methods may be totally unable to do so. When extending that to PDAEs, it is becoming more and more difficult and may completely stress the numerical method. For non specialists and even for specialists, PDAEs solving look like an inextricable numerical jungle. Because of this, it appears a lack of universally applicable solution methods in spite of the current effort.

Among the large number of numerical methods devoted to the solution of PDE or PDAE systems which are by nature very difficult to solve, a well established classification would be the following ones.
Numerical methods may be based on :

- the use of Method of lines (MOL) (Carver,1981 ; Schiesser, 1977, 1991)
- Finite difference Methods (Anderson and al., 1992)
- Weighted Residuals Methods (Finlayson, 1980 ; Villadsen and Michelsen, 1978)
- Finite Element Methods (Strang and Fox, 1973 ; Carey and Finlayson, 1975)
- Finite Volume Methods (Pantakar, 1980)
- Adaptive Grid Methods (Verwer and al., 1989 ; Arney and Flaherty, 1990)
- Moving grid Methods (Pilipis, 1990 ; Miller and Miller,1981)

As mentioned previously, all of them are of interest, with pros and cons on a numerical point of view.
MOL , basically convert PDEs into sets of DOE with respect to time by involving space discretization. The main advantage results in that sophisticated framework based on well established methods [LSODI, (Hindmarsh, 1977) ; DASSL (Petzold,1982), DASOLV(Jarvis and Pantelides, 1992), RESEDA (Le Lann and Sargousse, 1993, 1997)] may be used for large set of DOEs or DAEs. But as main drawback, general DOE or DAE solvers have difficulties to control and estimate the impact of the space discretization error on the general numerical scheme, especially when coarse spatial grids have to be used.

The most interesting feature of the finite volume formulation is that the resulting solution ensures that the conservation of quantities involved such as mass, momentum and energy is exactly satisfied not only over any group of control volumes but over the whole computation domain, which is not the reality when dealing with finite difference methods.

Finite element approach takes advantage in that ability to divide domain of interest in elementary sub-domains, namely elements. It may therefore handle problems with steep gradients and may deal with irregular geometric configurations.

Adaptive and moving grid methods seem to be the most promising in the fact that the idea is to use a numerical method in which nodes are automatically positioned in order to follow or anticipate deep fronts. It may be done by using two basic strategies, namely the spatial redistribution of a fixed number of points and the local grid refinement. The principal advantage of this method is that the original grid structure is preserved, but at the detriment of computer time and storage increase. More, as mentioned in Brenan and al (1989), coding of such techniques is relatively difficult and may throw complex problems as discontinuities, frequent restarting of the numerical methods.

When looking to the most recent literature and as mentioned by Oh (1995) in its attempts to propose a general framework under gPROMS (Barton and Pantelides,1994 ; Oh and Pantelides, 1996) dealing with modelling and simulation of combined lumped and distributed processes, the aim of constructing reliable software capable of solving a wide spectrum of PDE/PDAE/IPDAE problems has not yet fulfilled and even does not look reachable in the nearest feature. Some reasons for that (Machura and sweet (1980) ; Oh (1995))

- PDE problems allow a considerable freedom of formulation
- some specific features of PDE problems require very specific treatment
- There exist so many numerical methods designed to deal with small classes of problems, none of them being truly universal.

Despite this pessimistic view, constant effort have been developed into two main directions : Domain-specific packages designed to deal with a particular physical problem domain such as CFD (Computational Fluid Dynamics) with typical CFD package such as PHOENICS (Cham, 1987), based on finite volume techniques, FLUENT, ESTET, POLY3Dand General-purpose packages. such as PDECOL (Madsen and Sincovec, 1980), DSS/2 (Schiesser, 1977, 1991). High-level PDE packages such as PDEDIS (Pfeiffer and Marquardt, 1993) have to be mentioned also in this context.

In conclusion of this part, which has been particularly devoted to the PDEs background, it may be notice that problems of interest to process engineering are usually described as PDAE systems, even as IPDAE systems when dealing with population models (Ramkrishna, 1985 ;. Toutain and al ; 1998). More, these dynamic models try to be

the most « high fidelity » models used and applied in realistic operational environments. It means that they may be used in various configurations such as abrupt changes, start-up and shutdown configurations,...
These models should further be used for simulation, including parameter estimation, even in the near future for fast real time computing. It may involve in realistic environment the necessity of state events detection, treatment of internal discontinuities (change in model mode : single phase to two or three phase systems such as in plate-fin brazed heat exchangers) and external discontinuities due to deep change on feed or on operation parameter.

According to that, the most pragmatic approach seems to be that belonging to the MOL approach with two stages as suggested by Oh (1995). A rough sketch of it is presented on figure 1.

At first, PDAEs are discretized in terms of finite dimensional representations, using the « ad hoc » discretization schemes (finite differences or finite volume approach in order to insure balances conservation). By the way, PDAEs are transformed into DAEs with respect to time. Then, DAEs are integrated using appropriate integration techniques with time and state events detection.

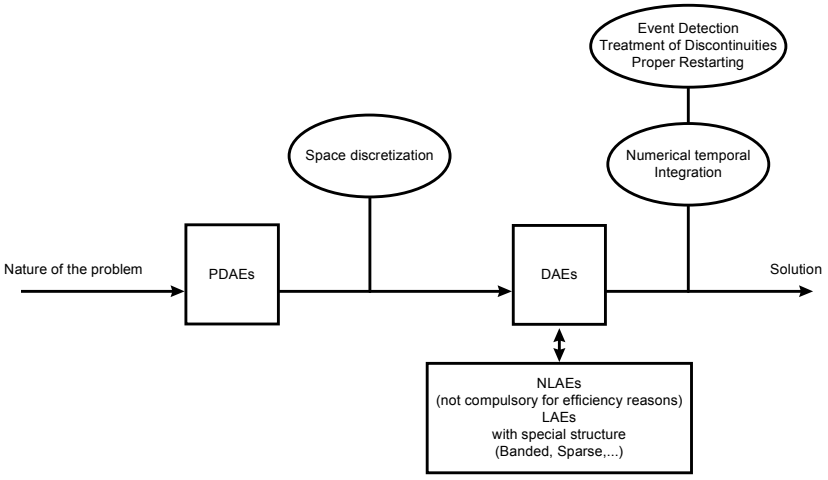

Figure 1 : Numerical strategies for PDAEs for robust Dynamic Simulation

In order to illustrate the proposed methodology, it will be presented two different types of applications which will give a real idea of subjects treated, despite the non universality of the framework.

2. DYNAMIC SIMULATION OF WASTEWATER TREATMENT PLANTS BASED ON BIOFILTERS

Basically, biofilters may be assimilated to a packed bed column, where biological reactions and filtration phenomena occurred. Their main advantages are their high compacity and efficiency for biological epuration (carbon, nitrogen, phosphorous), their good integration in the environment (no noise, no smell), their low energy consumption and sludge production. Inside the bed, carbon particles are retained physically by a deep filtration phenomena. At the same time, micro-organisms settled in the support act as biological catalysis in order to promote biological reactions to remove pollutants. In case of denitrification, they transform NO_3 to NO_2 and finally to N_2. As a result, biomass is growing inside the bed and contribute to the clogging of the biofilter.

The dynamic simulation of these kind of processes is very useful for model validation, performance investigation, parameter estimation and control strategies development with automatic process management in mind. In this context, a dynamic mathematical model for submerged granular bed biofilters has been proposed. It is presented in a general form and can be used for many different applications (denitrification, carbon removal, nitrification, denitritation...). Knowing the basic biological and physical phenomena, macroscopic balances equations are written and lead to a system of non-linear partial differential and algebraic equations (Jacob and al., 1997) which

has been solved by two different numerical approaches.

2 1. Global resolution using the Method of Lines (MOL)

The problem to be solved may be written in vectorial form with adequate initial and boundary conditions :

$$D(s,t)\frac{\partial s}{\partial t} = f(s,t,u,p) + g(s,t,u,p)\frac{\partial s}{\partial z}$$

With generalization in mind, a numerical strategy inspired by differential and algebraic equations (DAE) treatment associated to a space discretization using the method of lines is applied. It allows :
- a global treatment of the system without discrimination between the variables (especially for algebraic ones).
- a treatment of the physical model in its original form, as it was written, without preliminary manipulations.
- the use of sophisticated methods which has been developed for initial value differential-algebraic equations.
- the possibility, for further works, to use the developments involved in DAE systems (parameter estimation, sensitivity analysis...).

The main failures of the method are the large size of the resulting DAE system obtained after discretization (this problem can be reduced by using adequate numerical conditioning of the system) and the rigidity of the fixed grid discretization scheme which is not really a problem in our case (because their is no sharp space profiles) and could be solved by using a moving grid approach.

The numerical method of lines consists of a discretization for the spatial variable (vertical position z) in N discretisation points. Each state variable **s** is transformed into N variables corresponding to its value at each discretization point. The spatial derivatives are approximated using finite difference formula on 3, 5 or 7 points (the best results for accuracy and computation time efficiency were obtained with 5 points).

The resulting N x n DAE system is solved by Gear's multistep and multi-order implicit method based on a predictor-corrector scheme]. At any time step, a non-linear system has to be solved in the corrector loop. The Newton-Raphson method is used for a quick convergence and because we have a good initialization with the predictor. The derivatives are computed analytically in the dynamic operator which has a block structure. Each block is an n x n matrix corresponding to the model equations at one discretization point. The extra-diagonal terms come from the spatial derivatives approximation. Thus the dynamic operator is a multi-diagonal block matrix and we gain memory space accuracy and computation time saving by treating it like a banded matrix, transforming it to a rectangular matrix for which the pivot research is done vertically.

As the biofilter is cleaned when the pressure drop reaches an upper limit, a procedure to detect automatically state events and automatic restarting has been implemented. It has allowed to treat start-up configurations after each cleaning of the biofilter In case of time events, polynomial approximations are used to simulate flow-rate and concentration input variations without introducing discontinuities.

2.2 Resolution with an Orthogonal Collocation Approximation Approach

In the field of process control based on the use of infinite dimensional models, a compromise between the low model complexity and the high solution accuracy has to be found. That's why, after the global resolution method presented before, a functional approximation method is used to obtain a state representation with a low finite dimension with a satisfying accuracy.

As presented previously, the dynamics of the process is described by a non-linear distributed parameter model. The partial differential equations of the model are reduced to ordinary differential equations (solved by using Runge-Kutta integration method or Gear's method for DOE) by using an orthogonal collocation method (Villadsen and Michelsen, 1978).The choice of this method for the space discretization of the biofilter model has been dictated by two main reasons. First of all, this method is largely used and accepted in chemical engineering (Jorgensen, 1986) for the reduction of dynamic models of tubular reactors ; secondly orthogonal collocation is known to be an efficient and powerful method, provided some precautions are respected about the choice of base functions and others parameters. Moreover, it offers the advantages that its implementation is easier, that the nature and the dimension of the state variables remain unchanged after the reduction procedure and that it is conservative for mass and heat balances.

The collocation method consists of expanding the variables as a finite sum of products of time functions and space

functions.

$$s(z,t) = \sum f_i(z).C_i(t)$$ with N number of collocation points

The first question to be put is : how can we choose the base functions $\mathbf{f}_i(z)$ and the right value for N ? Polynomials are the most usual choice, preferably orthogonal polynomials, avoiding ill-conditioning matrix in the resolution. In what follows we choose the Lagrange interpolation polynomials, defined through (N+1) points and satisfying an orthogonality condition.

It has been shown that the best approximation is obtained when the collocation points are used as interpolation points. Moreover the best collocation point location corresponds to the zeros of orthogonal polynomials such as Jacobi polynomials $P_N^{(a,b)}$:

$$\int_{z_0}^{z_L} (z - z_0)^{\beta} (z_L - z)^{\alpha} z^j P_N^{(\alpha,\beta)} dz = 0$$

Both parameters a and b are considered as optimisation parameters of the collocation point location. The best choice depends on the nature of the model. It has been shown (Cho and Joseph, 1992) that, for non-linear systems, it's better to place the collocation points where the non-linearity is more pronounced. In general, the approximate solution accuracy increases with the collocation point number. In fact, we showed that the model accuracy depends more on the collocation point location than on their number; inappropriate values of a, b and N lead to numerical instabilities.

2.3 Application to a denitrification filter ($NO_3^- \rightarrow NO_2^- \rightarrow N_2$)

In order to dissociate nitrates and nitrites, two distinct biological reactions are considered in the model : denitratation ($NO_3^- \rightarrow NO_2^-$) and denitritation ($NO_2^- \rightarrow N_2$).

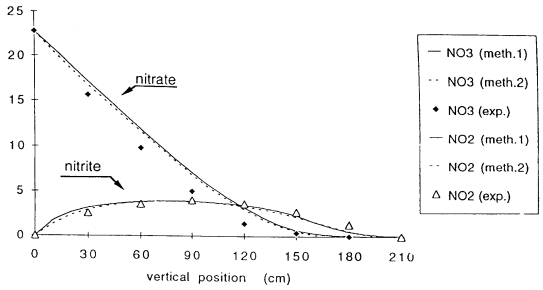

Fig. 2 : NO_3 and NO_2 profiles (mg N-No_x / l)

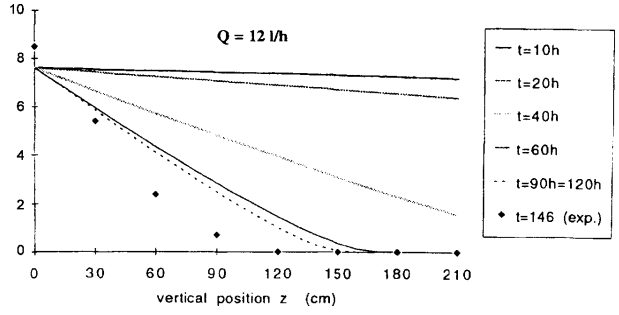

Fig. 3 : Nitrate profiles in the filter (mg N-NO_3 /l)

The two methods (Meth1 : MOL + DAE ; Meth2 : Collocation + DOE/DAE) give equivalent results and a good simulated/experimental data agreement for nitrites/nitrates and carbon concentrations is obtained (Fig. 2 and 3). On a numerical point of view, the two methods used to reduce the distributed parameter model to a DAE system (method of lines and orthogonal collocation) give similar results, in an equivalent CPU time which in fact is not really in favour of the collocation method, which should be , on a theoretical point of view, faster.

In the further control development based on a reduced model (Bourrel, 1997), the collocation method, leading to a

smaller dimension system, has been used but the global method has remained necessary to validate the model reductions and to know how far it may be reduced without losing in consistency : the problem consists in finding a good compromise between low complexity and high accuracy of the model. . Then, collocation methods has appeared to induce in the numerical scheme some instabilities, in part due to the non linearities to the system and to the increasing stiffness. On a practical point of view, despite the interest of this method, it has been replaced by a difference finite method which didn't present such kind of erratic behaviour.

This project is an interdisciplinary project under the auspices of MIDIGEP-Environment between INSAT (Unité de Recherche Procédés biologiques : Dr E. Paul), LAAS-CNRS (DR. J. P. Babary), LGC-UMR 5503 (Groupe d'Analyse Fonctionnelle des Procédés : J. M. Le Lann). It has been supported by the French Ministry of Research and Technology and by the Midi-Pyrénées Region (CCRRDT). It is involved in the European COST 682 project untitled : « Optimizing the design of biological wastewater treatment plants through the use of computer programmes based on a dynamic modelling of the process »

3. DYNAMIC PROCESS SIMULATION OF THERMAL CYCLIC ABSORPTION PROCESS (T.C.A.P.)

3.1 The T.C.A.P process

The T.C.A.P. process (Thermal Cyclic Absorption Process) is a novel approach in order to separate hydrogen isotopes by the way of selective absorption on Palladium (Horen and Lee, 1992). It is a semi-continuous process or an hybrid system with a succession of continuous operation and multiple state events. By the way, it presents some challenges for proper and optimal operability and for further process control studies. It is actually an experimental project at C.E.A. One of that major quality : it didn't need any pump device for fluid flow which is crucial when dealing with radioactive or nuclear components such as deuterium or tritium. In the subject of this paper, it will be applied to the separation of Hydrogen and Deuterium (H_2 - D_2).

On a descriptive point of view, it is composed by two basic components :

a chromatographic column of separation with a double heat-exchanger shell for heating and cooling. This column is filled with Alumnae Palladium pellets.

a capacity (storage tank) full at the beginning with pure Hydrogen, called inverser.

This process is performed via a cyclic operation. Each cycle will be divided in six steps as shown on Figure 4.

1. Feed loading : a small quantity of mixture H_2/D_2 to be separated is introduced in the middle of the column, initially cold.
2. Separation phase : the pure hydrogen in the inverser is introduced at the top of the column. Due to the Palladium selectivity in regard with the lighter hydrogen isotopes, the Hydrogen is preferentially absorbed on the solid pellets and throw away the Deuterium at the column bottom.
3. Heating phase : the column is isolated (all valves are closed) which induces an increasing pressure.
4. Side-stream phase : the Hydrogen is removed at the top and, at the same time, the Deuterium is collected at the bottom.
5. Desorption phase : the remaining H_2 in the column is send back to the inverser by flashing.
6. Cooling phase : the entire column is cooled and a new six step cycle may start again.

All along the cycles, this pure Hydrogen initially contained in the inverser is little bit polluted by Deuterium (for example, after thirty cycles, there is 15 % of Deuterium in the inverser).

By some analogy, this T.C.A.P. process may be considered as a class of regenerative processes which are fairly common in chemical and environmental engineering applications. Although it is generally not too difficult to design loading, separation steps,... separately it is much more complicated to design and operate an entire process cycle when the end of the absorption phase is in fact the beginning of the desorption one. Small changes or deficiencies during one step may influence on one cycle, can accumulate from cycle to cycle and then strongly affected the cyclic operation and the hypothetical « cyclic steady state » which is unreachable due to the progressive pollution in the process. This type of reactor-separator also called multifunctional reactor has been recently used for

adsorption, ion exchange and regenerative heat exchanger. Some recent papers have discussed their importance (Salinger and Eigenberger, 1996) but focused on the determination of the « cyclic steady state ». More as proper design, scale-up and stability analysis of cyclic processes requires a large experimental effort and long time practical experience, it has been decided in this contribution to focus on a direct dynamic simulation approach. It may provide a basic understanding of the process dynamics, allow to study the cyclic multiphase operation and to perform stability analysis. By increasing parameter sensitivity and parameter determination, it allows to apply sequential experimental approach in order to reduce experimental effort.

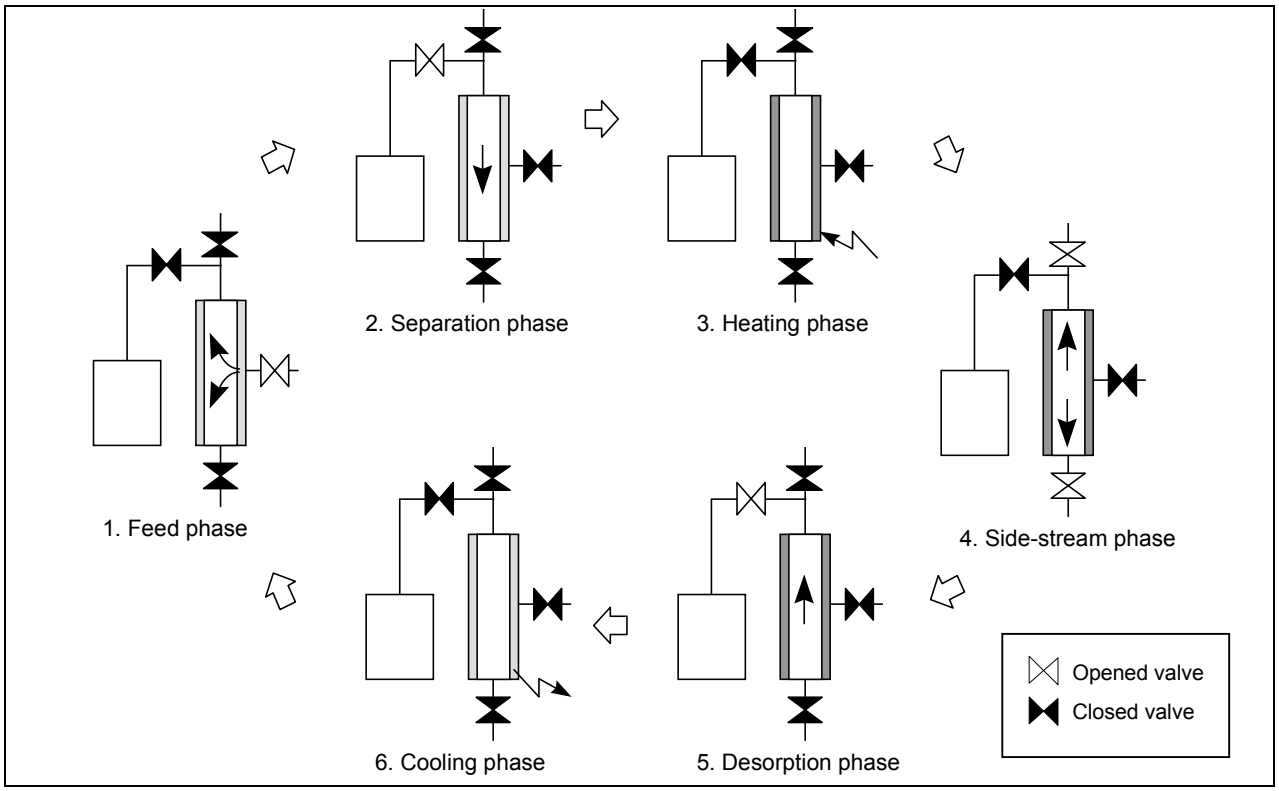

Fig 4 - T.C.A.P. process

3.2 Dynamic modelling

This proposed model (Sargousse and al., 1997) is based on mass and energy balances, (including equilibrium equations for absorption, isotopic separation) and pressure drop calculation. As special feature, it takes into account the modelling of hysteresis phenomena.

3.3 Numerical strategy

The complete modelling for the T.C.A.P. process leads to a system of partial differential and algebraic equations . It involves multiple time and state events detection in order to take into account the sequencing multi-step phases which are part of the processing. It can be handled by state of the art simulation approach for systems of algebraic and partial differential equations in time and one spatial coordinate. However, after using methods of lines (MOL) with different difficulties due to the erratic behaviour of the solution, as well as the reverse velocity which may appeared everywhere at any time all along the column, a finite volume scheme with fixed grid has been adopted for spatial discretisation. This has allowed to insure the conservation of balances which was not with MOL based on difference finite scheme. The resulting set of DAE system has been solved using the efficient and robust framework developed in this field (RESEDA (Le Lann and Sargousse, 1996)°: a panoply of integrator solvers, originally based on Gear's method implemented by Hindmarsch (1980) which has been extended in order to solve index 2 DAE problems with initialisation consistency and discontinuity handling applied to very large complex problems). In the particular case of the TCAP dynamic simulation, it has induced the detection of time and state events, the detection of discontinuities, the proper restarting of the method and the automatic calculation of initial consistent values.

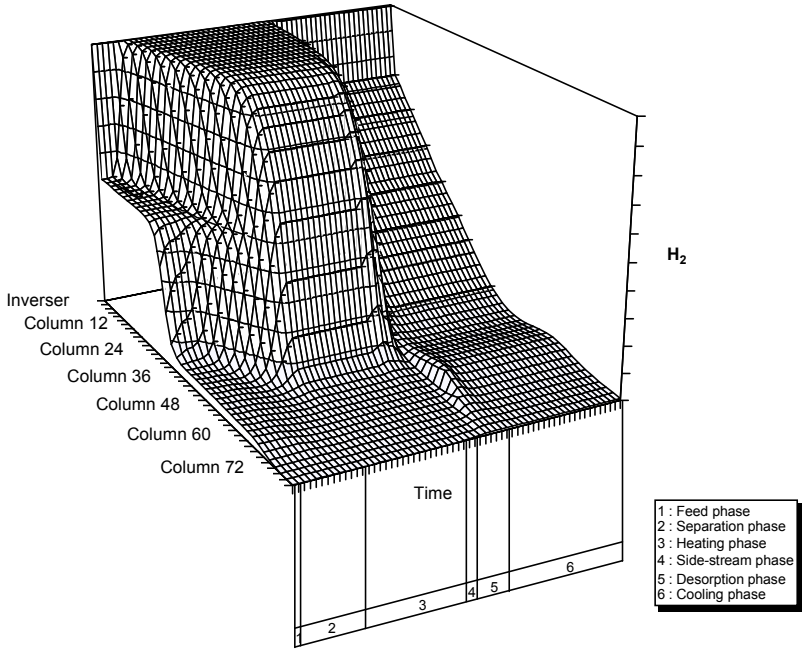

Fig. 5 : A 3D view of some results

This project has been the result of a fruithful collaboration between the « groupe d'Analyse Fonctionnelle des Procédés »(LGC-UMR 5503 : A. Sargousse, J. M. Le Lann, X. Joulia), the CEA-DAM-Centre d'é&tudes de Valduc (D. Leterq) and ProSim S.A. (P. Sere-Peyrigain)

4. CONCLUSIONS AND PERSPECTIVES

In this paper, after focusing on a theoretical point of view on different ways to solve PDAEs, some experiments with their success and inherent difficulties have been briefly presented.

The proposed methodology, in spite its non universality seems to be a fruitful one in the context of a general framework for Process Dynamic Simulation.

It is currently applied on others research projects : one devoted to the dynamic simulation of catalytic three phase reactors for hydrogenation (Julcour and al , 1998) in collaboration with the Multiphase reactors team (Prof. H. Delmas and A. M. Wilhem, LGC), one dedicated to the dynamic simulation of plate fin heat exchangers (in collaboration with Nordon Cryogénie), one for the dynamic simulation of reactive absorption column based on rate-based approach for VOC removal (Rascol and al ., 1998) in collaboration with the Simultaneous Energy and Mass Transfers team (Prof. M. Prevost), and two others dedicated to the solving of IPDAEs (integral partial Differential Algebraic equations). One for the dynamic simulation of liquid-liquid Extraction pulsed column based on Maxwell-Stefan approach coupled with drop population model (J. Toutain and al., 1998) in collaboration with the solvent extraction team (Prof. C. Gourdon, Prof. G. Casamatta) and the last one on the modelling of Batch cristallisation (F. Espitalier and al., 1997) in collaboration with the crystallization and precipitation team (Dr B. Biscans).

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