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General Purpose Dynamic Process Simulator Based upon the Cluster-Modular Approach

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Abstract

The objectives of this work are to present the dynamic simulation strategy based on cluster-modular approach and to develop a prototype simulator. In addition, methods for the improvement of computational efficiency and applicability are studied. A process can be decomposed into several clusters which consist of strongly coupled units depending upon the process dynamics or topology. The combined approach of simultaneous and sequential simulation based on the cluster structure is implemented within the developed dynamic process simulator, MOSA(Multi Objective Simulation Architecture). Dynamic simulation for a utility plant is presented as a case study in order to prove the efficiency and flexibility of MOSA.

1. Introduction

Dynamic simulation has been accepted as a powerful tool to predict unsteady state behavior of chemical processes and can be used in all phases of process engineering activities such as process design, operation, control and automation. In recent years, the world-wide process industries are now focusing their attention on dynamic simulation to improve the design and operation of plants, process control systems and process safety systems. Much of the work is concentrated on process modeling (structure, representation and tools), numerical techniques (higher-index problems, consistent initialization, etc) and advanced simulation environment(software integration, user interface, etc)(Marquardt, 1991).

Up to now, various approaches for solving the equations of the dynamic model of processes have been discussed and implemented. There are two distinctly different methods for dynamic simulation: equation-based and module-based approach. The integration strategy of a large set of mixed differential and algebraic equations is the most essential issue in dynamic process simulation. In fact, there are many possible computational strategies to solve the equations of dynamic model. The advantages of module-based approach are;

- ease of understanding and implementation,
- the maximum size of computational block is determined not by the total unit but by the largest unit,
- improvement of computational efficiency by parallelism of process.

The disadvantages of this approach are;

- poor convergence and efficiency when a process has strong interactions,
- the need of synchronization or coordination when different integration methods are adopted to different modules.

The advantages of equation-based approach are;

- flexibility in problem definition,
- convergence not affected by recycle stream.

The disadvantages of this approach are;

- the need of large computer memory,
- the need of structural problem formulation,
- the need of advanced numerical methods.

It is desired to combine the advantages of above two approaches. In this paper, a cluster-modular approach which has a simultaneous integration capability is presented and the general purpose dynamic process simulator, MOSA is described.

2. Cluster-modular approach

The module-based approach can be classified into two types of simulation methods according to the role of a numerical integrator: simultaneous and independent modular method (some authors refer to these as coupled mode and uncoupled mode). In the former a common integrator is used to integrate differential equations of all modules simultaneously, whereas in the latter each module can have its own integrator. A whole process can be partitioned into several blocks according to flowsheet structure or dynamics. After precedence ordering of these blocks, it is possible to get sequential computational structure. If the block is solved simultaneously, the whole process can be solved without tearing dynamic coupling.

2.1 Simulation model

The model equations representing any unit of chemical process can be classified into three groups: first-order ordinary differential equations(ODEs) representing the balance equations(eq. 1), a set of internal algebraic equations(eq. 2, 3) and a set of coupled algebraic equations(eq. 4). The internal algebraic equations include only internal algebraic variables, x, which are defined only in the module, whereas the coupled algebraic equations include external algebraic variables, z, which are defined in the other module.

$$\frac{dy}{dt} = f(y, x, z, d, t) \qquad (1)$$

$$x_i = g_i(y, x_i, x_e, d, t) \qquad (2)$$

$$x_e = g_e(y, d, t) \qquad (3)$$

$$x_c = g_c(x, y, z, d, t) \qquad (4)$$

Here, y is ODE state variable, x and z are algebraic variables, d is design parameter and t is time. If ODE model(Gani et al., 1990, 1992) is used to solve the above equations, all ODEs of a cluster are solved simultaneously by a common integrator and then each module is in charge of solving algebraic equations in the sequential modular fashion.

2.2 Three-phase calling procedure

An inexact coupling may be introduced when eq. (4) is solved, since the external algebraic variable, z, may not be updated. To avoid this problem, following three-phase module calling procedure is suggested.

Phase 1 - Solving the internal algebraic equations: To solve internal algebraic equations, each module is called by integrator through interface. After this stage the value of all internal variables of each module are known. It is expected that many of external variables, z, may be calculated.

Phase 2 - Solving the coupled algebraic equations: To solve coupled algebraic equations each module is called by integrator.

Phase 3 - Evaluation of right hand side of ODEs: Through phase 1, 2, all variables are available to evaluate the r.h.s. of eq. (1).

Although above three-phase calling procedure copes with many types of practical simulation problems, it is difficult to have exact coupling when the form of eq. (4) is $x_c = g_c(z_c, \ldots)$. This often occurs when the modern complex control scheme is introduced. The only weakness of the modular approach presented is sequential treatment of this true coupling algebraic equations. A direct substitution is implemented in the developed simulator to overcome this disadvantage. In fact, it was reported that this iteration scheme is stable and has no special difficulties in dynamic simulation(Ponton, 1982). Therefore general 3-phase calling procedure is used: $1\text{-}2^M\text{-}3$ calling procedure (The phase 2 calculation is forced to do M times where M is small integer, usually, 2 or 3).

3. The MOSA system

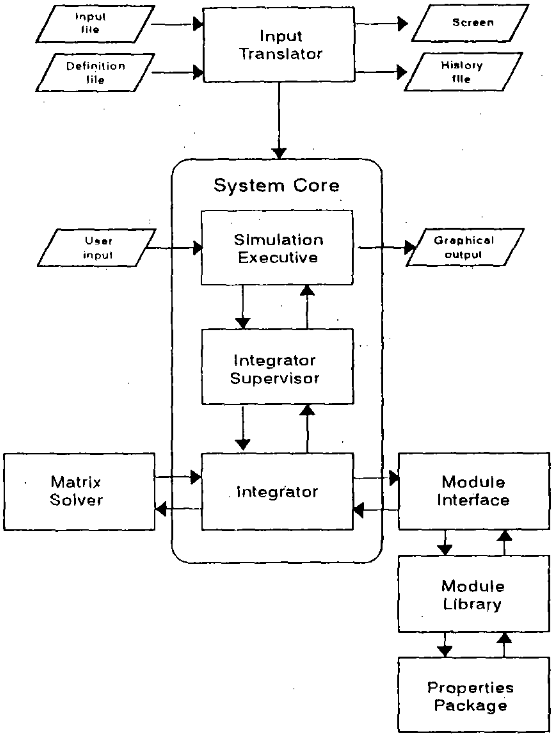

Fig. 1 Architecture of MOSA.

3.1 An overview of MOSA

MOSA is a module-based process dynamic simulator which has simultaneous integration capability and employs highly flexible structure for various application areas including discrete process simulation such as batch process.

The main components of MOSA are shown in Fig. 1. The characteristics and functions of each component are as following:

· Input language system

The input language system interprets the keyword-oriented input file and then generates simulation problem by writing main drive routine, event routines and data. Also, this pre-processor analyzes the flowsheet structure and generates a initial clustering structure by performing partitioning and precedence ordering. User can modify this initial clustering structure by adding his specific knowledge of the process.

· Executive

The executive monitors and controls the overall simulation task such as one step integration of overall problem, time and state event handling, interactive simulation, printing and display. Especially at run time, user can interrupt the simulation by pressing any key on the keyboard and communicate with the system.

· Supervisory integration routine

The supervisory integration routine is in charge of one- step integration of the whole problem.

· Equation solving package

The equation solving package includes stiff integrator, matrix solver, etc.

· Model library

The model library is a set of FORTRAN 77 subroutines which model unit operation blocks or computational blocks.

· Physical properties package.

The physical properties package has a physical property database of hydrocarbon components and subroutines for calculation of enthalpy, density, K-value through equation of states such as Soave-Redlich-Kwong, Peng-Robinson, etc.

Current version of MOSA is implemented using FORTRAN 77 on PC.

3.2 Sparse Jacobian handling

As the size of integration block increases, the Jacobian matrix become more sparse. Sparse matrix technique enables us to save storage and computing time. The sparsity pattern can be constructed analytically or by numerical differentiation. In this work, we obtain the Jacobian sparsity pattern by using sensitivity analysis based on the numerical perturbation. Using this pattern, the variables are grouped to reduce the computational burden of Jacobian evaluation by finite difference method.

3.3 Discontinuities handling

Various discontinuities can be introduced in dynamic simulation. Typical reasons for discontinuities in process model are phase change, control variables change by digital control system or a switch from a certain model equation to more appropriate one during a transient. Furthermore a process may have inherent discontinuities due to discontinuous process operation. These are typically encountered in batch processing and in continuous processes in start-up or shut-down operations.

In this work, MOSA finds discontinuity time using interpolation of discontinuity equation when a discontinuity condition is satisfied.

3.4 Event processing

Many discrete events are included in applications of dynamic simulation, for example, batch process, start-up, shut-down operation, etc. For these discrete events the concept of event and state is used. An event is something that happens at a point in time, such as equipment trip and operation change and the state of the system is changed to new state by event. A state diagram can be represented by a graph whose nodes are states and directed arcs are the transitions labeled by event names. An example of a state diagram is shown in Fig. 2 and event section of input file, in Fig. 3. Events have condition and action statements. The type of condition statement is either implicit or explicit. Some authors refer to these as state event and time event(Barton, 1994). For an implicit event, the time of the occurrence of the event(discontinuity) is not known. On the contrary, for an explicit event, the occurrence time is known. And the type of action is either point or duration. If the condition is satisfied, point action is taken once at that moment. Duration action is a continuous action taken during the time when the condition is satisfied.

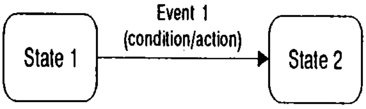

Fig. 2 State and event diagram.

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SECTION EVENT
   Boiler_Trip IN CLUSTER 1
   TYPE = EXP , POINT
   COND = ( TIME - 60. )
   ACTION ( NB = 4.0 )
```

Fig. 3 Event section.

4. Case study

The utility boiler process of a refinery plant, which consists of 5 boilers including control system, was simulated using MOSA. The process model consists of 11 unit blocks and has 19 ordinary differential equations and 118 variables. Fig. 4 shows the block diagram of the utility boiler plant. The key function of a utility boiler plant is to supply high quality steam stably; hence the pressure of header should be controlled tightly. The level of a drum should also be controlled to guarantee safe operation. The objective is the improvement of operability and safety through dynamic simulation of expected faults or situations.

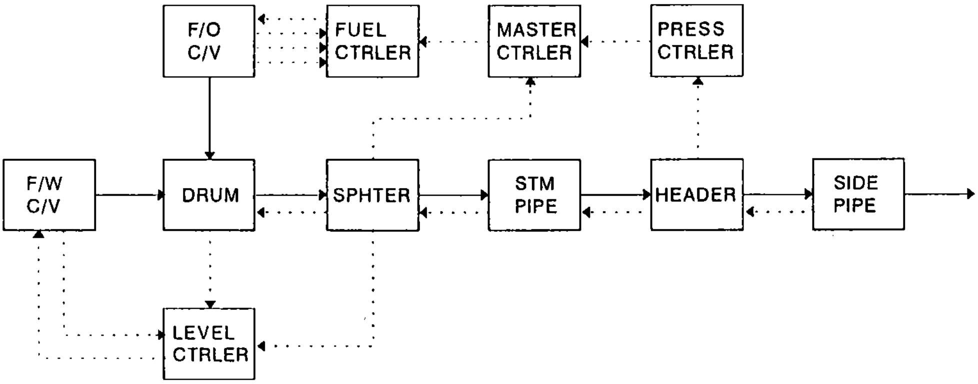

Fig. 4 Block diagram of utility boiler plant.

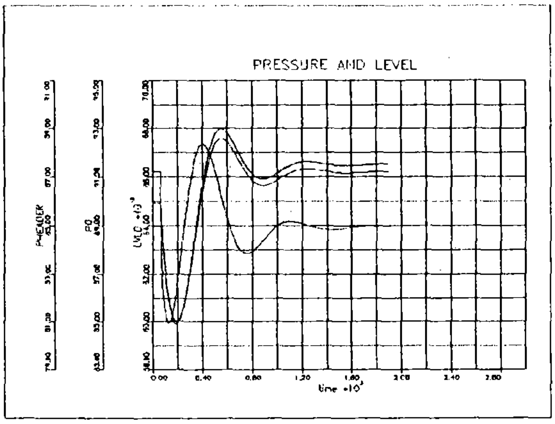

Fig. 5 Pressure and level.

The simulated situation is the trip of one of the 5 boilers and the simulation time is 60 minutes. Fig. 5 shows the pressure of high pressure header and level of boiler drum versus time. In this figure, the pressure and the level reach a new steady-state after about 60 minutes.

5. Conclusions

The general purpose dynamic process simulator, MOSA, based on cluster-modular approach is presented. The architecture of MOSA is adaptable to various problems and application areas. Currently, the expansion of model libraries, structural modeling techniques and applications to real plants is being studied.

Acknowledgements

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