INTEGRATING WORKFLOW EXTENSIONS INTO A PROCESS-INTEGRATED ENVIRONMENT FOR CHEMICAL ENGINEERING

Michalis Miatidis[1] and Matthias Jarke[1,2]
[1]Informatik V, RWTH Aachen, 52056 Aachen, Germany
[2]Fraunhofer FIT, Schloss Birlinghoven, 53754 Sankt Augustin, Germany

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Abstract: Design is one of the most complex and creative tasks undertaken by chemical engineers. The early production stages of chemical design require an adequate support because of their critical impact on the competitiveness of the final products, as well as their environmental impact. In cooperation with researchers and industries from the chemical engineering domain, we have created an integrated flowsheet-centered environment for the support of the early stages of design. In order to address the global need for enterprise integration observed in today's highly competitive global economy, we had to make our system more aware of further organizational aspects of the executed processes. As a solution to this challenge, we integrated a number of workflow extensions into our environment. These extensions enabled it to provide its method guidance further across the inter- and intra-enterprise environment of our enacted processes, with the future goal of seamless interoperating with other external systems of the overall enterprise environment. In this paper, after capturing the rationale behind the need for this integration, we successively describe the integrated environment and detail the extensions employed. Finally, we illustrate our approach on a small case study from our experience.

1 INTRODUCTION

The support of chemical engineering design processes is a very challenging task because of their creative nature and critical role in the overall production. They primarily include the original specification, simulation and evaluation of several design alternatives of a chemical product participating in a production lifecycle. It can be argued that these early stages have a great impact on most of the *sensitive* characteristics of the whole production like the final product *quality*, the *cost* of the overall investments and operations, as well as the *duration*.

We address the demand for supporting the early stages of design processes in chemical engineering in the *SFB 476 IMPROVE* research project (Nagl and Westfechtel, 1998). In this project, in cooperation with chemical and plastics engineering experts, we investigate the early phases of the polyamide6 production, the so-called conceptual design and the basic engineering. To this end, we have developed a process-integrated design environment that is able to directly provide the engineers performing the design processes with situated fine-grained process support based on previous recorded experiences (Jarke et al., 1999a). This environment is built on top of *PRIME (Process Integrated Modelling Environment)* (Pohl et al., 1999). PRIME process support is given in the form of *method guidance* based on the interpretation of method definitions of some well-known parts of the processes. Through a *process integration mechanism*, the behaviour of the participating tools is automatically adjusted according to the method definitions that apply to the current situation.

The contemporary business trends are clearly towards the need for a global integration, either within a company (*intra-integration*) or among several enterprises (*inter-integration*) (Vernadat, 1996). In order to keep our environment up to date with these changes in the manufacturing world, we needed to reflect the organizational nature of the enacted design processes in our environment by further addressing the internetworking issue of the engineers provided with support throughout supply chains. In pursuit of this goal, we have extended our initial approach with workflow extensions that reflect the more coarse-grained enterprise nature of process execution.

In section 2 we detail the motivation for this integration by successively comparing the workflow management support with the method guidance and describing the integrated modelling approach that has driven us. In section 3 we introduce our process-integrated design environment built upon PRIME and detail the extended metamodel adapted in pursuit of the integration goal, and in section 4 we illustrate our results on a small case study from the IMPROVE

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project. Finally, in section 5 we provide some conclusions and outlook to future work.

2 MOTIVATION

2.1 Workflow Management versus Method Guidance

Both *method guidance* and *workflow management* contribute to the support of processes being executed (figure 1). Nevertheless, each one of them supports the executed processes at a different level of granularity and from a different perspective. They differ in three main aspects:

- The primary concern of workflow management is the *process-centric* automated coordination of the interworking of human actors at the execution level. In contrast, method guidance aims at directly supporting the human actors performing these activities by defining their detailed *methods of working*.
- The products considered by workflow management and method guidance vary in their granularity. The process logic of a workflow model considers the products at the *level of documents*. Method guidance, on the other hand, cares of the *product structure* of these documents as they are considered in a more fine-grained level by the method definitions.
- Workflow activities are bound to a number of resources that perform some work on behalf of them at runtime. These resources mainly contain the participating human actors, tools and computer systems. Since method guidance is *restricted* to some activity performed by a human actor at an engineering workplace, the main resources it considers are the involved tools.

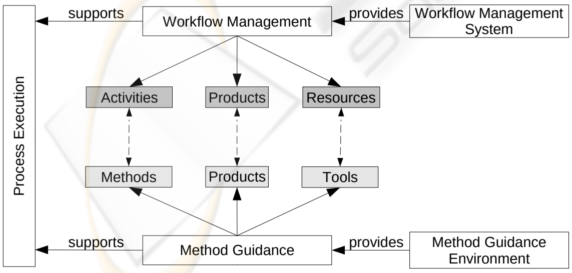

Figure 1: Two levels of support to process execution.

The need to provide process support and automation to the execution of business processes, has lead to the appearance of a variety of workflow management and method guidance standards utilized by large enterprise information systems. The area of workflow management stems from the traditional area of *office automation* solutions. These solutions were oriented to the automation of office processes performed by human actors. Most of the modern approaches have been widely applied in banks, insurance companies etc to manage organisational issues of routine processes most of the times with no or little human intervention (van der Aalst and van Hee, 2002).

In the area of method guidance we can identify the traditional *handbooks* that have dominated the industrial practice, to the more modern separate *guidance tools* displaying to the user a list of valid method definitions that apply to his given situation, e.g. (Nuseibeh and Finkelstein, 1992).

None of the above solutions is able to provide a fully integrated method guidance being at the same time aware of the enterprise coordination issues, without underestimating the non-determinism of the involved processes. Workflow management systems provide technical support for the automated coordination of processes that are supposed to be precisely known in advance. Most of the researchers of this field focus on the workflow management support and the possible ways of integrating it with the higher level of project management or enterprise resource planning (ERP) e.g. (Cardoso et al., 2002), (zur Muehlen and Rosemann, 2004) but neglect the method guidance to the human actors performing the processes. On the other hand, the existing method guidance techniques are concerned with short-lived methodologies that deal with individual activities or participants and neglect other more managerial and organisational activities. A gap clearly exists between the two levels of support that has not been adequately investigated in the literature and needs to be bridged.

2.2 Integrated Modelling Approach

Workflow management supports the executed processes based on the explicit definition of a *workflow model* capturing the process logic. On the other hand, method guidance is specified in process models capturing the *method definitions (methodology)* for performing a task. Thus, method definitions provide a *zoomed view* of workflow activities and detail the ways of working of the human actors performing them. Also, the products and resources are seen as black boxes on the task level and are zoomed to their structure on the method guidance level. The resources are actually considered only on their tools by the method definitions. As a consequence, we can defined three ‘*semantic bridges*’ among the interrelated elements of the two levels:

1. A *mapping relationship* between a workflow activity and the methods providing guidance to the en-

gineers during that activity execution.

2. An *isA* relationship from the products (documents) of the workflow model to their detailed view on the method guidance level.
3. An *isA* relationship from the tools belonging to the resources of the workflow model to their detailed descriptions on the method guidance level.

We have defined an integrated modelling approach that is based on these semantic bridges and integrates the interrelated concepts of the two levels of support. In figure 2, a 3-dimensional view of this approach is presented. The upper part represents the *workflow management level* and the lower part the *method guidance level*. On each one of them, we can identify the contributed concepts. On the upper, we have the *activities*, the *products* manipulated by them and the involved *resources*. On the method guidance level, we identify the *engineering methods*, the *products* they change and the involved *tools*.

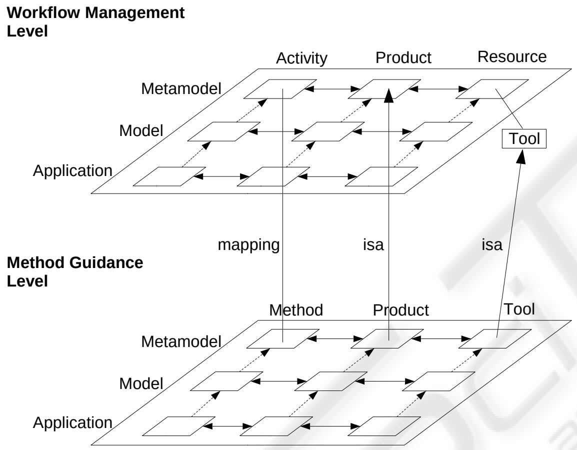

Figure 2: Integrated modelling approach.

In order to provide a generic modelling formalism that is powerful enough to capture a wide range of design scenarios and not restrict to just some specific cases, we have followed the *IRDS standard* (ISO/IEC, 1990) and have created a three-layered hierarchy for each level as shown in figure 2. The *metamodel layer* plays the role of a generic kernel which is *domain-independent*. Due to the generality of its underlying concepts, it can be applied in different creative domains of design. The *model layer* provides the domain-specific knowledge of specific design scenarios by instantiating the metamodel level entities. In other words, the model layer provides a description of the ideal world. The real world is captured on the *application layer*. This layer instantiates concepts of the model layer and captures traces of the actual process execution. The two modelled levels are integrated defining *static relationships* on the metamodel level for each semantic bridge among the relevant elements.

In the next section, we present the PRIME-based design environment that has been extended according to our integrated approach. Since PRIME was already providing the fine-grained method guidance support, we followed a bottom-up approach and extended its metamodel with elements from the coarse-grained workflow management level according to the three aforementioned semantic bridges.

3 PROCESS-INTEGRATED DESIGN ENVIRONMENT

3.1 The PRIME-based Flowsheet-centered Architecture

PRIME is able to provide integrated method guidance to engineers based on the reuse of traced experiences. The core component of PRIME is a *process engine* that provides process support (automation, guidance or enforcement) based on the interpretation of method fragments and product object schemata, maintained in a *Process Data Warehouse (PDW)* (Jarke et al., 2000).

The method guidance is provided to the user through a *process-integration mechanism* (Pohl et al., 1999) of the engineering tools. Process-integrated tools are able to *adapt* their behaviour according to the current enactment state and actual method definitions (*process sensitivity*), provide support to the engineers for direct invocation of method fragments and return feedback information on service execution.

The capabilities of the process-integrated tools are explicitly defined in tool models and are integrated with process models providing the *method guidance definitions*. Processes are modelled using a situation-based contextual metamodel, initially proposed in the *NATURE project* for the requirements engineering process (Jarke et al., 1999b). A user is at any time in a subjectively perceived *situation* made of a set of states of the products undergoing the development. In every situation, he has a given *intention* in his mind and the conceptual bridge between a situation and the valid intentions is called *context*. Contexts can be further refined to *executable*, *choice* and *plan* contexts. Executable contexts automate pieces of a process and are usually realized by tool functions,choice contexts describe the need of the engineer to make a decision among several alternatives and plan contexts define a systematic plan of steps that the engineer has to follow. Tools are modelled with respect to their capabilities (actions exposed and graphical user interface elements) with a tool metamodel. The two metamodels are integrated into the *environment* metamodel (lower part of figure 4).

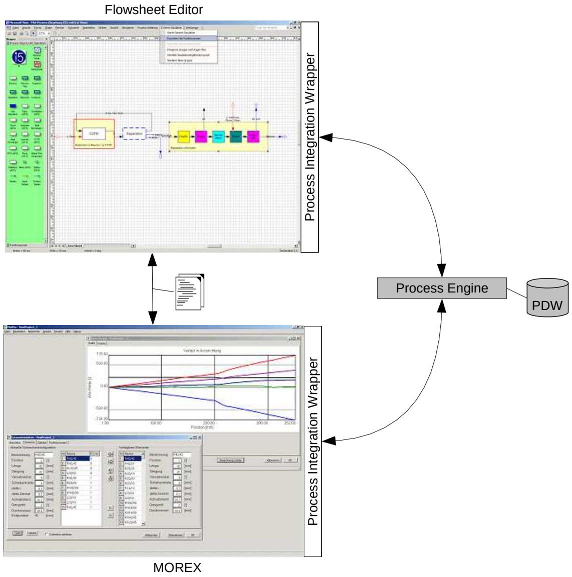

Figure 3: Integration architecture.

We have built our integrated design environment on top of a flowsheet-centered PRIME architecture. We have realized a novel flowsheet editor (Bayer et al., 2001) on the basis of the Microsoft Visio commercial drawing tool. Through the process integration mechanism, we have defined method fragments modelling the basic interaction patterns of the engineers while working on flowsheets. Some of the features we stressed were the ability of displaying different refinement alternatives to the user and the simultaneous display of different refinement abstraction levels in the same flowsheet view.

In order to make the data of the flowsheet accessible from outside, integration with other domain-specific tools was demanded. This exchange of information among heterogeneous tools, is supported by special *integration tools* (Becker et al., 2002) that, under the supervision of the process engine, ensure data consistency between documents. Figure 3 shows a part of the actual integration architecture which integrates the central flowsheet editor with the *MOREX* (Schlüter and Haberstroh, 2002) compounding extruder simulation tool. Contrary to our flowsheet editor, MOREX was *loosely* process-integrated as it already provides hard-coded method guidance to the engineers and thus the process engine guidance was limited.

3.2 Extended Metamodel

Our goal was to extend our original PRIME process metamodel and integrate it with workflow elements according to our aforementioned integrated modelling approach. To this end, we adapted metamodel extensions according to the *Workflow Management Coalition (WfMC)* Standard (WfMC, 2001). WfMC has developed specifications for standards that concentrate common characteristics of workflow management products. As a result, these specifications improve the opportunities for the effective integration of commonly used workflow concepts and thus promote the interoperability with other workflow products. The resulting metamodel is shown in figure 4. The existing NATURE metamodel is shown at the lower part of the figure and is divided by a dotted line with the adapted extensions shown at the upper part.

Following the WfMC reference metamodel, the pieces of works that have to be done are captured in the *activity*. An activity represents a logical unit of work that requires the support of human and/or machine resources for its execution. An activity can be arbitrary complex and be iteratively composed of others until the basic activity level is reached. In our extended metamodel we call the activities *tasks* in order to emphasize their assignment to human actors.

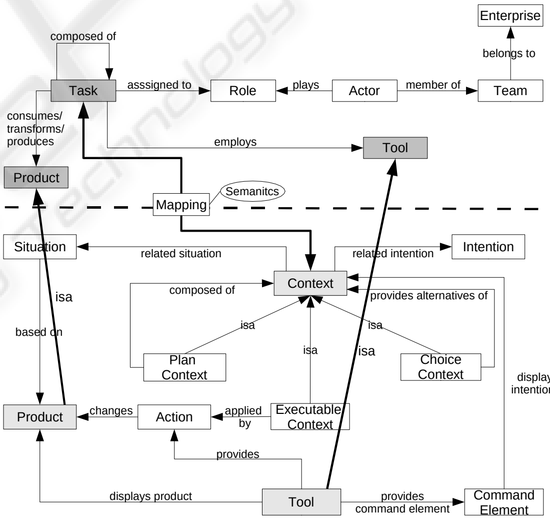

Figure 4: Extended environment metamodel.

A task provides the virtual world inside which method guidance according to method definitions is provided. Thus, it makes sense to create a *semantic mapping* between tasks and NATURE-based contexts reflecting the methods. This mapping *(first semantic bridge)* represents the methods that define the legal *ways of working* of a human actor during the enactment of a task. The mapping may also be carrying some *semantics* for providing important shared knowledge such as time scheduling information, a partial order in the engineering contexts or even define the contexts that signal the beginning or the termination of the task execution.

While a task is being executed, it produces, consumes and transforms *products*. The products produced by a task are characterized as output products of the task, and the products consumed are characterized as input products. Input products of a task can be either existing products from other project sessions or output products of other predecessor tasks. On the task level, the products are considered as documents flowing from one task to the other. On the contextual level, the structure of the products is detailed to allow methods to change their properties. As a result, an isA relationship exists among them *(second semantic bridge)*.

Each task requires a number of *resources* in order to be carried out. Resources include primarily the *human actors* assigned to them, their enterprise settings and the employed *tools*. Actors are indirectly associated to their assigned tasks via their roles. Roles are distributed according to the knowledge background, skills and assigned responsibilities of the actors playing them. Actors can be divided into *teams* belonging to *enterprises*, that work synergetically for the achievement of a common goal. Since method guidance is provided directly to a specific actor who is performing a specific task at a specific workplace, the resources considered on this level are *restricted* to the involved tools. Similarly to the case of products, tools on the method guidance level are detailed with respect to their capabilities and an isA relationship is also here deduced *(third semantic bridge)*

With the above metamodel extensions and the three semantic bridges, we have managed to increase the PRIME *awareness* of the more coarse-grained levels of process execution. As a consequence, PRIME is able to extend its method guidance mechanism for the inter-activity support of different human actors. The benefits of our approach are illustrated on a small case study in the next section.

4 CASE STUDY

In this section, we detail a small example based on a case study from the IMPROVE project that illustrates the benefits of our approach. For the reasons of simplicity and understandability, we use a small and simplified fragment from our overall polyamid6 scenario.

Polyamid6 is produced from monomer chemical plants. The design process consists of three prominent process steps: reaction, separation and compounding. We are going to focus on the *compounding phase*. The compounding process modifies the polymer in order to give it some desired characteristics (such as heat resistance and mechanical stability). Two expert roles contribute to this process: the *compounding expert* and the *1D-simulation expert*. The main task of the compounding expert, is the conceptual configuration of the compounding extruder inside the process-integrated flowsheet editor. The resulting configuration is further analyzed by the 1D-simulation expert who simulates the compounding extruder configuration based on physical and mathematical models.

Because of the integrated workflow extensions, PRIME is able to further apply coordination and method guidance *outside of the frontiers* of a specific task. Process engine is aware of the interconnected tasks and through the semantics of the mapping of contexts to activities, contexts signaling the beginning or the termination of a task can be known. Thus, in the case of a need of control and data flow among two activities, the terminating context of the first task, can be coupled with the beginning context of the second through a plan context and the data transfer can be realized under the support of the process engine.

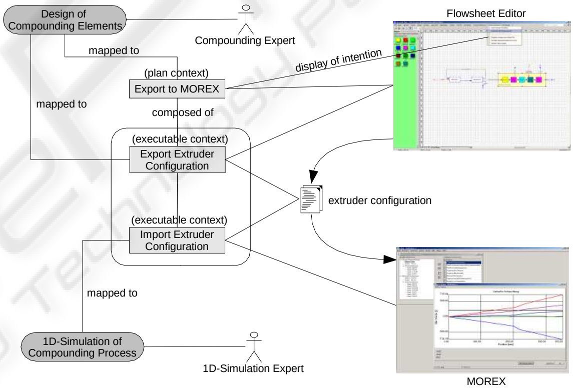

Figure 5: Example of inter-activity method guidance.

Figure 5 shows a UML-like diagram of the transition from the ‘*Design of Compounding Elements*’ task of the compounding expert to the ‘*1D-Simulation of Compounding Process*’ task of the 1D-simulation expert. The compounding expert is invoking the ‘*Export to MOREX*’ plan context through a menu item in the flowsheet editor. This plan context defines the strategy (steps) for the transition. The first step is the executable context ‘*Export Extruder Configuration*’, applied automatically by a flowsheet editor action, that exports the extruder configuration to XML format. The next step is the ‘*Import Extruder Configuration*’ executable context applied by a MOREX action in the workplace of the 1D-simulation role. It receives the exported extruder configuration and imports it in MOREX creating a new project configuration. Now the expert can modify the properties of the received extruder if needed and start the simulation.

5 CONCLUSIONS AND OUTLOOK

In this paper we presented the extensions applied to a PRIME-based environment for supporting chemical engineering design processes. Initially this environment was capable of providing intra-activity situated method guidance i.e. at a specific engineering workplace. Motivated by the integration trends in modern enterprises, we developed a modelling approach extending our existing fine-grained process models and integrating it with the more coarse-grained level of workflow activities. This integration was achieved using the three introduced semantic bridges. As a consequence, the gap between the workflow management level and the method guidance level was narrowed. A better understanding of the full granularity spectrum of the executed processes was achieved and our environment was able to further provide inter-activity method guidance to various engineers.

Our adapted integrated modelling approach, concentrates two viewpoints on our executed processes. On the method guidance level, our contextual process model captures method fragments and thus views processes '*in the small*'. On the workflow management level, on the other hand, a broader view is taken decomposing processes to well-defined tasks. In the near future, we are planning to investigate ways of further capturing inside our underlying models the intermediate level of methods as *assemblies* of our stored method fragments (Ralyté and Rolland, 2001).

Further future work is planned to address the area of interoperability of our integrated environment with other external components of the IMPROVE integrated design environment. In particular, we are interested to integrate our fine-grained method guidance environment with the *AHEAD reactive administration system* developed for the coarse-grained management of design processes (Westfechtel, 2001). Our main goal is to enable AHEAD to directly call the PRIME process engine services such as direct manager-triggered invocations of specific process fragments and to get back notifications concerning the execution status of activities.

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