ABSTRACT
This paper introduces high-throughput screening of biological samples in life sciences, as a domain for analysis of human-robot interaction (HRI) and development of usable human interface design principles. High-throughput screening (HTS) processes involve use of robotics and highly automated analytical measurement devices to transport and chemically evaluate biological compounds for potential use as drug derivatives. Humans act as supervisory controllers in HTS processes by performing test planning and device programming prior to experiments, systems monitoring, and real-time process intervention and error correction to maintain experiment safety and output. Process errors are infrequent but can be costly. Two forms of cognitive task analysis were applied to a highly automated HTS process to address different classes of errors, including goal-directed task analysis to describe critical operator decisions and information requirements and abstraction hierarchy modeling to represent HTS process devices and automation integrated in screening lines. The outcomes of the analyses were used as bases for generating supervisory control interface design recommendations to improve existing system usefulness and usability.

Categories and Subject Descriptors
I.3 [Life and Medical Sciences] – biology and genetics.

General Terms
Performance, Design, Experimentation, Human Factors.

Keywords
High-throughput screening, human error, cognitive task analysis, goal-directed task analysis, abstraction hierarchy modeling.

1. INTRODUCTION
Within the past decade, biological and chemical screening processes, which have historically been carried out by human operators, as part of life science operations, have become increasingly automated (see [14]). Time-consuming operations, such as pipetting (transferring) liquid extracts of compounds into micro- (culture) plates, mixing compounds with reagents, etc. are now performed by robots, with the goal of increasing throughput, as well as enhancing test accuracy and promoting operator safety. As a result, the role of human operators in this domain has changed dramatically from manual material handling tasks to planning, controlling and analyzing the results of automated screening lines.

Contemporary high-throughput screening (HTS) processes involve chemical-based assays of organic and inorganic compounds for effects on human cellular functions, or enzymatic reactions that are common in cells [6]. Among the uses of HTS is the testing of compounds that may have the potential to serve as bases for drug derivative development for use in future medications for treating cancer, viruses, etc.

At the University of Rostock (Germany), Center for Life Sciences Automation (CELISCA), marine compounds undergo enzyme-based (e.g., Trypsin) testing in order to identify compounds that might be useful for such drug development (“hits”). The compounds being tested are typically from organisms that are able to survive in extreme conditions in the Baltic Sea, including highly polluted environments. Such organisms are selected as candidates for testing because they may provide compounds to create pathways in human cells for dealing with dangerous bacteria and toxic agents.

Assaying compounds involves several major steps, including: pipetting liquids (enzyme substrates, test compounds, reagents) at different quantities and concentrations into micro-plates; incubating micro-plates in order to elicit enzymatic reactions at temperatures similar to those that occur in the human body; and analyzing the reactions using optical colorimetric measurements.

Full automation of the enzyme-based screening includes integration of an optimized robot for chemical analysis (ORCA) with analytical measurement devices on a process line. The robot, which is custom designed for the screening process, can be configured for specific experiments. The integrated devices include: a robotic-based barcode print and apply device for labeling and tracking the micro-plates in which compounds are tested; an automated pipetting robot and system for filling micro-plates with liquids; an incubator for controlling the temperature of reactions in the micro-plates; and an automated micro-plate reader for analyzing the enzyme activity, or cellular reaction, in each plate well using luminance or fluorescence tests of light reflected off samples (see Figure 1).
The (barcode) print and apply device integrates a mobile micro-plate holder that is capable of precise rotation and positioning of plates along horizontal and vertical axes for accurate positioning of labels. This robotic capability makes human programming of labeling operations complex. The ORCA, which is programmed, controlled and monitored from a central process control system (PCS), transports micro-plates to and from the various workstations on the screening line. The PCS also manages the coordination of machine activities (controlled by their own local controllers). Each line has the capacity to process several hundred organic compound extracts as part of a single experiment. Typical production volumes include thousands of samples processed over 2-3 day periods.

3. HUMAN-ROBOT INTERACTION IN HIGH-THROUGHPUT SCREENING

Specialized biological screening tests, such as the Trypsin enzyme-based assay, are developed by biochemists and published in the biochemistry literature. These publications describe “bench-top” versions of tests; that is, they describe how to manually perform a particular screening assay. At CELISCA, biopharmacologists adapt the manual bench-top protocol of the screening tests to automated HTS lines in state-of-the-art laboratories. This involves:

- identifying the appropriate micro-plates to be used in the automated assay;
- determining the configuration of liquids within each micro-plate;
- selecting automated devices to be used to perform the assay (e.g., deciding whether a centrifuge will be needed to create solutions of reagents in plate wells);
- planning the pipetting processes (e.g., which tips and reservoirs will be used by the robot); and
- establishing an optimal sequence of assay steps.

After developing the automated screening test protocol, operators program the pipetting robot using specialized software to carry out sequences of actions such as removing a micro-plate lid, pipetting liquids from a reservoir to the micro-plate, replacing the lid, and dispensing used pipetting tool tips. The plate reader also has its own proprietary control software and is programmed to run the necessary analytical measurements. These devices, as well as the barcoder and incubator, are integrated through the PCS using a screening line “method editor” application. This application communicates with the user interfaces of the proprietary device software through an “executive” software controller. The method editor includes standard Windows action/configuration dialogs for all devices on the HTS line, which are used to set parameters and to send data to device software modules via the executive controller. The editor is also used by operators to create methods, which resemble flow diagrams that describe the screening test in terms of micro-plate movements among the different workstations.

Following the initial HTS method development, a pilot run is initiated to evaluate system performance in terms of the correctness of chemical reactions, precision of robot motions, etc. If the run is successful and the results are accurate (i.e., comparable to manual assay results), the screening test is ready for execution on batches of compounds. After the completion of each assay, operators ascertain whether results meet predefined quality criteria and analyze the data according to client demands. The steps to developing, controlling, and analyzing an automated assay for HTS are summarized in Table 1. The table identifies the functions of the human operator and the HTS automation for each step.

One supervisory controller typically operates the HTS process by planning and programming robotic tasks. An additional lab technician works on delivering micro-plates, chemicals, plate labels, pipetting resources, etc. to the process line. Although there are some health and safety risks for technicians in such tasks, the operations are currently handled by humans because existing automated guided vehicle technologies are not considered to be reliable or accurate enough.

Table 1. High-throughput screening assay steps.

<table>
<thead>
<tr>
<th>Step</th>
<th>Operator</th>
<th>HTS System</th>
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<tbody>
<tr>
<td>1.</td>
<td>Plan and design experiment</td>
<td>Pilot assay run</td>
</tr>
<tr>
<td>2.</td>
<td>Program pipetting robot</td>
<td></td>
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<tr>
<td>3.</td>
<td>Program plate reader</td>
<td></td>
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<tr>
<td>4.</td>
<td>Program methods for labeling micro-plates, preparing sample micro-plates, and preparing and analyzing test micro-plates</td>
<td>Assay run</td>
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<tr>
<td>5.</td>
<td>Monitor system; correct errors</td>
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<tr>
<td>6.</td>
<td>Ensure accuracy of pilot run results</td>
<td></td>
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<tr>
<td>7.</td>
<td>Edit automated assay method as necessary</td>
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<tr>
<td>8.</td>
<td>Monitor system; intervene in process control and correct errors</td>
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<tr>
<td>9.</td>
<td>Ensure assay results meet quality criteria</td>
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<tr>
<td>10.</td>
<td>Analyze data generated during assay run</td>
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<tr>
<td>11.</td>
<td>Repeat Steps 8-10 for each batch of compounds</td>
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</table>
A typical HTS experiment poses a high cognitive workload for supervisors, who must keep track of the timing of process steps, whether chemical reactions are occurring safely, and whether robot motions are accurate. Errors can occur at many different phases of the screening process. For example, in material handling, ORCAs may fail to pick-up labware from a line station or they may place a micro-plate at an incorrect position. These errors occur for different reasons, such as incorrect initial positioning of labware by operators or misalignment of robot position coordinates with the position of work platforms for test plates at analytical measurement devices. These types of errors develop in the automation programming and “start-up” phases of the HTS process. Errors can also occur at specific devices, such as the pipetting robot. They may include misalignment of the robot arm, hardware problems (e.g., loss of communication with the PCS), material-related errors such as pipetting tips falling off the robot gripper, and operator errors such as forgetting to prepare and place liquids at the pipetting robot workstation. Similar errors can occur at the other automated devices on the HTS line.

Beyond these specific device errors, chemical reactions may not progress as planned because of operator programming slips or mistakes in experiment execution or the wearing down of device components. This can lead to delays in reactions or the need to scrap an entire experiment. This is very costly to the test facility because many of the organisms being investigated are extremely rare and the extracts are expensive to develop. Therefore, operators may need to periodically intervene in the master robot control in order to prevent a line from “crashing”. The process control interface must provide the capability for near real-time, closed-loop programming of process events based on the progress of an experiment.

Although operator and system errors are rather infrequent, occurring approximately once every 75 assay runs, their cumulative effect can be substantial. Fixing an equipment or resource error, like replacing damaged pipetting tool tips on a liquid transfer robot or working through a series of error correction dialogs at the supervisory control interface for the HTS line, may only take a few minutes. However, other problems, such as a robot position error and collision with another line device, may require a process engineer to visit the line or purchase new parts. This type of problem can take several days to correct. Depending on the time needed to correct a problem, such errors can lead to delays in reactions or the need to scrap an entire experiment because of the limited life expectancy of biological compounds and enzymes.

4. COGNITIVE TASK ANALYSES

In order to address the potential for costly errors in human-robot interaction (HRI) in HTS processes, we identified the need to evaluate user goal states, tasks, and decision and information requirements. This analysis could then be used to make comparison with the capabilities of existing robotic and automated technologies for supporting user goal achievement. The objective of the evaluation was to identify functional limitations of HTS automated devices, like the robotic-based print and apply device, and potential usability issues with existing software control interfaces for programming, executing and analyzing screening experiments. Based on the success of cognitive task analysis (CTA) applications in many other domains (e.g., [7], [9], [15]) towards achieving similar objectives, we elected to use several specific methods in combination to support recommendations on HTS line design enhancements.

The behavior of biopharmacologists in planning, executing and analyzing results of HTS operations, as well as the lab automation and equipment that is used to facilitate these operations, can be identified through the use of CTA. In this research, we applied the methods of goal-directed task analysis (GDTA) and abstraction hierarchy (AH) modeling. The combination of AH models describing screening line devices and automation with the results of a GDTA on biopharmacologist performance of HTS operations can provide a meta-method for understanding how HTS operator task and functional requirements are currently addressed (or not) by the existing system components. Furthermore, information requirements identified through the GDTA, combined with specification of interface action sequences based on AH models, can be used to identify potential usability issues with existing software control interfaces. Thus, we used comparisons of the GDTA and AH models to formulate interface design and automation functionality recommendations for the existing software applications used in HTS.

This new integrated CTA approach may be applicable to many complex work domains; however, the information that can be gleaned from GDTAs and AH models in combination is particularly useful in HRI. HRI applications typically involve high workloads for human operators under time pressure, requiring them to maintain high levels of situation awareness (SA). For example, in HTS operations, biopharmacologists need to monitor robotic operations, address system errors and sometimes reprogram assay methods “on the fly” to ensure the success of an experiment. The SA requirements of supervisory controllers in this domain are extensive, informing elaborate robot programming decisions. The GDTA methodology was developed to reveal operator critical decisions and SA requirements in such complex domains, as a basis for supporting effective cognitive systems design [3, 8]. With respect to the utility of the AH modeling technique for the HRI domain, the method allows for detailed representation of complex system functions at many levels of abstraction and representation of modes of system operation. Scholtz, Antonishek and Young [13] offer that HRI is a complex domain that requires operators to interact with physical devices and real, dynamic environments. The HTS domain is one in which the state of the robotic hardware and analytical measurement devices may change from time to time, depending upon the needs of a screening method or specific task. A device representation, like AH modeling, allows operators to examine the functionality of systems, subsystems and components under different modes of operation and can ultimately be useful for promoting detection, analysis and recovery from dynamic error conditions.

CTAs have been used to analyze HRI tasks in the past. For example, Adams [1] describes preliminary work on a GDTA for the task of managing multiple robots in search and rescue operations; Usher and Kaber [13] developed a GDTA characterizing supervisory control of flexible manufacturing systems; and Ricks [12] proposes creating an AH model of robot teleoperation as a basis for an ecological interface (although no such model is generated). To our knowledge, few, if any complete, applications of GDTA in the HRI domain have been
reported and GDTA and AH modeling have not been used in concert in HRI or in any other domain.

4.1 Goal-Directed Task Analysis

GDTA is an information requirements assessment methodology developed by Endsley [3] which has been used in many prior CTAs (e.g., [2], [3], [5], [15]). A GDTA focuses on identifying operator SA requirements relevant to performing complex systems control. The steps to conducting a GDTA include identifying the users’ major goals, identifying subgoals to support the overarching goals, identifying operational tasks to achieve the subgoals, identifying questions as part of decision making in task performance, and developing information requirements to answer these questions (e.g., [15]). This information is elicited from a domain expert in structured interviews. The analyst then creates an outline (or goal tree) describing the information requirements, independent of the technology that may ordinarily be used to achieve task goals and subgoals. The results of a GDTA include lists of critical operator decisions and SA requirements that can be used as a basis for design of complex system information displays, operator selection, and developing training programs and SA assessment measures [4].

We developed a GDTA describing biopharmacologist goals, tasks, decisions and information requirements relevant to supervisory control of the HTS line. We conducted interviews with an expert biopharmacologist at CELISCA. The expert was provided with a general model of a goal tree for a GDTA, like that shown in Figure 2. She was provided with an explanation of how information or SA requirements were to be organized at three different levels, including perceptual knowledge requirements (Level 1), requirements for relating perceived system states to task goals (Level 2), and requirements for projecting future system states (Level 3). An analyst subsequently posed questions to the biopharmacologist to motivate breakdown of HTS process goals, tasks and identification of SA requirements at each level. Example questions included:

- What is the purpose of each major task to the present goal? (Why do you perform the task?)
- Is your concept of how this task is to be performed consistent with the standard operating procedure? (If not, how is it different?)
- What are the critical decisions you must make in completing the task?
- What pieces of information do you require to address each critical decision as part of the task?
- When do you need each piece of information during the task procedure (at what stages)?
- How are the various pieces of information related to each other?

Figure 2. Goal tree model for GDTA (courtesy Melanie C. Wright).

The complete GDTA resulting from this research on biopharmacologist adaptation of bench-top assays to HTS processes included 25 high-level goals, 20 subgoals, and a total of 88 tasks to these subgoals. On average, there were 4.4 tasks to each subgoal and 2.2 critical decisions per task. An analysis of the SA requirements associated with the biopharmacologist decisions revealed a total of 228 unique pieces of task information for planning, executing and analyzing HTS experiments. Since the complete GDTA is too large to be included in this paper, only two examples will be discussed here.

Figure 3 presents a section of the GDTA outline, as part of discovering compounds leading to drug derivative development, for a specific goal (1.1.9.1), which deals with automated application and reading of barcode labels during the HTS process. This goal involves two tasks: (1) integrating the print and apply device into the process (using the PCS software); and (2) determining how it will be used during the assay. Two decisions must be made by the operator when integrating the barcoder: (1) what information will be included on the label?; and (2) where will the label be applied to a micro-plate? The information required to address these decisions is the code that will be used on the label. To achieve the second task of determining the functions of the barcoder, the operator must decide whether a new barcode needs to be applied to micro-plates or whether an existing barcode is to be read. In addressing this decision, the operator needs to know whether a barcode is already present on the micro-plates (from the manufacturer or client) and what step is to follow bar coding in the assay process. To facilitate data collection (using the micro-plate reader), for example, it is first necessary to record the content of the barcode label.
4.2 Abstraction Hierarchy Modeling

Abstraction hierarchy (AH) modeling is the representation of a work domain model in an event-independent manner in order to promote operator ability to recover from unanticipated error conditions in working with complex systems [16]. The errors that were described for the HTS process at CELISCA represent good candidates for this type of analysis. AH models are hierarchical, structural models consisting of multiple levels of abstraction [10]. At the highest level, the models define the purpose of technology in the work domain. At the lowest level, the physical components of the system are represented. Generalized functions of the system are shown in between. Linkages among the levels ("means-end connections") represent how the purpose of the system is implemented through specific devices and they also provide an explanation of why certain components are needed to achieve a system purpose [11].

AH modeling has historically been used in complex work domain analyses, including anesthesiology, process control and nuclear power plant control [7, 10, 11]. This methodology has been found to be an effective tool for: revealing how automated system functions are facilitated through specific components; establishing the frequency of use of specific system functions in operational scenarios; and establishing levels of information processing that may not be sufficiently supported by existing technology. The results of AH modeling can serve as a basis for developing automation interfaces for helping operators manage system states, when coupled with information on task strategies and operator decision making.

The example HTS process Goal 1.1.9.1 described earlier (facilitating micro-plate labeling and reading; see Figure 3) is supported by the barcoder device integrated on an HTS line. Figure 5 presents the AH model for the print and apply device. In general, this device is far more complex than a simple barcode scanner and requires programming and monitoring during specific steps of the assay process. The method for developing the AH models in the current study involved structured interviews with an expert process engineer at CELISCA to elicit device and automation purposes and functions. In addition, visits to the HTS line were conducted to inspect the existing technology.

In the upper-left corner of the diagram in Figure 5, the high-level goal or purpose of the device is represented. The next level down in the model identifies the constraining processes for the device, including labeling and reading barcodes. Below this level, the generic functions for the device are identified, including printing and applying barcodes. At the same level in the model, the generic functions are broken down into component processes (e.g., the processes for printing include feeding labels and printing foil, and applying thermal material from the foil to the label). The next lower level in the model is the physical component and function level. Here the subsystems required to complete the printing, applying and reading functions are identified. At the same physical function level in the model, the subsystems are broken down into components. The level of detail of the model is limited based on expert and analyst determination of what component knowledge may be critical for operators to understand equipment functions and to be able to diagnose faults, etc. Following the links from the top of the AH diagram down to the bottom, an operator can discover how the functions of micro-plate labeling and reading are implemented by the barcoder. Following the links from the bottom of the diagram to the top, an operator can learn why the various subsystems or components as part of the barcoder, such as the printer and the label paper feeder, are necessary for the specific functions of micro-plate labeling.

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**Figure 3. GDTA Goal 1.1.9.1 and associated tasks, decisions and information requirements.**

Figure 4 presents another section of the overall GDTA, which describes a portion of the goal of automating the manual bench-top screening test, namely the task of programming the pipetting robot. Operators must make four decisions in order to complete the identified task: (1) which pipetting tools to use; (2) how many pipetting transfers are necessary; (3) how to deliver liquids; and (4) the order of delivering solutions to micro-plate wells. To address these decisions, there are several information requirements: the configuration and components of the available devices, the available tip types, the volume of liquid to be transferred, and the location of source and destination wells.

**Figure 4. GDTA Task 3 of Goal 1.1.7 and associated decisions and information requirements.**

**1.1.9 Develop program for assay method using HTS line control software:**

1.1.9.1 Facilitate plate labeling and reading:

- T1 Integrate barcoder and reader into method.
  - What type of information content is to be included in the label?
  - What label position is to be used?
  - Need – Meaningful code representing plate content.

- T2 Determine functions of barcode device to be used during assay.
  - Does the assay require reading or print and apply functions?
    - Need – Presence of barcode on plate.
    - Need – Step in assay method that comes next (e.g., data collection).

**Figure 5. GDTA Task 3 of Goal 1.1.7 and associated decisions and information requirements.**

1.1.7 Adapt manual pipetting steps to automated version of assay:

- T3 Using pipetting device software (e.g., Bioworks®), program liquid transfer from stock solutions contained in deep well plates to sample plates (e.g., using Biomek2000®).
  - Which pipetting tools should be used for each step?
  - How many pipetting transfers are necessary?
  - How should the liquid be delivered?
  - Which order of wells will solution be delivered to?
    - Need – Configuration and components of available devices.
    - Need – Types of tips available.
    - Need – Amount of volume that will be transferred.
    - Need – Source and destination wells according to protocol and previous configuration of plates.
In this research, AH models were developed for all automated devices and robotics integrated in the HTS line at CELISCA, including the automated pipetting robot, incubator, ORCA (material transport robot), and automated micro-plate reader. In addition, AH models were created for all proprietary software and action/configuration dialogs, as part of the PCS software that allowed for specific device configuration and manipulation. We adapted the AH modeling methodology to represent software for controlling devices on the screening line under study.

4.3 Generation of Design Recommendations

To formulate interface design guidelines for enhancing the existing software applications, all GDTA goals that required task performance with the current software were identified. The AH automation models relevant to the identified goals were then used to establish lists of interface actions that operators would need to perform to achieve the goals. The existing software, as described by the AH model, was systematically examined for features or functions not supportive of operator goals and components that were inadequate in terms of usability. When an aspect of the existing software that did not support the usability or functionality required by an operator goal (according to the GDTA and interface actions spelled-out based on the AH model) was identified, a design recommendation was generated.

As an example of the outcomes of this method, in order to assist biopharmacologists in their decision-making in programming the barcode device, it was recommended that the software suggest to the user a default label configuration for printing and applying a new barcode, based on previously defined and stored label configurations in a database. It was also recommended that based on the presence of an existing barcode on the micro-plate, the system would suggest the appropriate action for handling the micro-plate; that is, printing and applying a new barcode versus reading an existing barcode. Such an enhancement to the existing software could also serve to warn operators of micro-plate misalignments before they cause a robot “crash” if the system detected a misplaced barcode when attempting to read it, this would indicate that the micro-plate position was incorrect in the plate holder, which would cause a crash if not taken care of. Similar recommendations were formulated for all other goals in the GDTA that pertained to the use of software or devices. (A more complete coverage of these recommendations is to be published elsewhere due to space limitations.)

Several modifications were ultimately made to a new prototype interface for the barcoder action/configuration dialog to address...
the recommendations described here and enhance its usability. For example, with the prototype, users are able to select one of several different label types and then drag-and-drop the label onto a rotatable pictorial representation of a micro-plate in order to specify its location. This is far more efficient than programming plate holder rotations and offsets using text entry fields for proper label positioning. The interface then prompts the user for the label content, based on previously stored labels. The interface, in general, is more intuitive, with obscure terminology removed and functions reorganized, based on common user tasks.

5. CONCLUSIONS

The domain of high-throughput biological and chemical screening presents many interesting opportunities in terms of HRI research. In this environment, users operate highly automated, complex systems involving multiple robots that interact with each other. Operator requirements are twofold: first, to plan and program HTS experiments based on manual tests; and second, to monitor the system for errors, such as robot “crashes”, which are costly to the test facility in terms of time and resources. These tasks pose a high workload for operators and their interaction with the system is not well supported by existing interfaces.

We employed GDTA along with AH modeling to characterize the knowledge structure of biopharmacologists in planning, executing and analyzing the results of high-throughput organic compound screening operations, as well as the lab automation and equipment used in these operations. Combining the results of these CTA methods provided a better understanding of operator needs and how they are addressed by existing technologies. In addition to this, identification of automation and system interface design limitations was facilitated. Results of these analyses were used to formulate usable interface design and automation functionality recommendations for the existing software applications. These results can also be used as a basis for initial design and prototyping of supervisory control interfaces that might be used by HTS operators for programming, monitoring, controlling, and analyzing multiple screening lines performing simultaneous assays.

Two caveats to this work should be noted. First, the analysis described above was carried out for a specific HTS operation, namely, testing biological compounds for their potential to serve as drug derivatives. This testing procedure requires the use of highly specialized robots, devices, line configurations, etc. However, other tests that are possible with an HTS line, such as chemical agent characterization, may make use of different line setups and control software programming. Biopharmacologist goals and tasks will vary in different tests, as will the method of automation, requiring the construction of a new GDTA and additional AH models for analysis of each type of operation. Thus, the generalizability of this work is limited. Second, a CTA is a time-consuming process. The knowledge acquisition and documentation phases involved in creating GDTAs and AH models are laborious, as is the formulation of interface design suggestions, based on the results. This requires the analyst to become intimately familiar with the domain, including operator tasks, activities and the tools of the trade.

The work described in this paper is part of an ongoing project to analyze and develop advanced supervisory control interfaces at CELISCA. The redesign recommendations formulated based on the CTAs are currently being implemented in the prototyping of novel interfaces for device-specific and general HTS method programming. Domain experts, including the biopharmacologists at CELISCA, will evaluate the usability of these prototypes, as compared to the existing software.

It is expected that the CTA methods used in this research could be applied to user and autonomy evaluations in other HRI domains (e.g., human supervisory control of multiple robots in flexible manufacturing systems). It is also anticipated that the interface design recommendations made through this research may generalize to other domains in which complex supervisory control interfaces are also used for managing interactions of multiple autonomous agents in high-speed operations.

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7. REFERENCES


