Title: Real Time Data Acquisition, Theoretical Modeling, and Adaptive Control of Batch Dyeing Processes

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Relevance to NTC Goals:

Goal 1: Research

Our project has made considerable progress over the past year toward long-term goals. In assessing our current status, we now re-assert the following long-term goals. Short term goals for year three have been included in the request for third year funding.

Our general long-term objective is to continue to explore novel methods of data acquisition, dye system modeling, controls development and process optimization in batch dyeing. To accomplish this, we have formalized the following specific research goals for the Dye Applications Research Group:

1. Evaluate state-of-the-art sensors and data acquisition devices for batch dyeing operations for the following characteristics:

   - accuracy
   - precision
   - robustness
   - applicability
   - speed of data acquisition

2. Where necessary, develop new sensors and techniques for (1) above.

3. Develop computer data handling techniques based on standard protocols for use in real-time control and post-process analysis, including theoretical modeling of batch dye processes.

4. Develop and evaluate new parametric and non-parametric control strategies through computer simulations and actual laboratory, pilot plant and N scale commercial batch dyeing experiments with the following characteristics:

   - real time
   - adaptive
   - multi channel I/O strategies
   - loss function minimization
   - robust

- rapid
- generally applicable
- simple enough to implement commercially

The novelty of the DARG approach is to interactively control the process to a **performance** specification, e.g., shade, rather than a process specification, e.g., temperature.

5. Develop parametric theoretical dye models which:

- interact with parametric control strategies in (4) above
- increase our knowledge of dyeing
- can be used to **"train"** non-parametric control **strategies**
- aid in experimental design and determination of parameters

6. Develop computer-related hardware to accomplish the above and evaluate that hardware for:

- **performance**
- feasibility
- robustness
- applicability

Goal 2: *Education*

1. Develop human resources (educated graduate students and research assistants) and new knowledge

2. Develop new science and technology

3. Publish results in appropriate journals

4. Sham research information with interested parties through technical presentations

Goal 3: *Partnership*

1. Foster continued and new partnerships with interested parties, especially as they relate to continued research and emerging technology transfer activities

   The cooperative effort between the Colleges of Textiles and Engineering continues to study and improve batch dyeing control systems. This work was initiated six years ago when the Consortium for Research in Apparel, Fibers, and Textile Manufacturing **(CRAFTM)** was **formed.** The combination of fundamental chemistry and engineering principles has led to innovative and significant improvements in monitoring, modeling, and controlling discrete dyeing processes.

   Collaborative efforts between our project and Ciba have also been productive and synergistic. Through an informal agreement, the Dye Applications Research Group **(DARG)** and Ciba have cooperatively developed the flow injection analysis **(FIA)** system to monitor individual dye concentrations in dyebaths. Ciba supported a summer graduate internship to improve **FIA** performance and has allowed Dr. William Hunter to lend his considerable expertise in analytical chemistry to the project, Dr. Hunter, an adjunct member of the Textile Engineering, Chemistry, and Science faculty, regularly attends biweekly DARG meetings, has served as a member of **Michele** Lefeber's MS. Advisory Committee, and continues in the same role on her **Ph.D.** committee. **In** addition, Ciba has provided detailed composition information about dyes that **are being** used in the theoretical modeling portion of our work. Without this cooperation from a major **dyestuff** manufacturer, our research would not have progressed as rapidly as it has.

Interest from major textile manufacturers has provided us with valuable feedback and encouragement A visitors book has been placed in the lab so that the number of people exposed to our research results can be monitored. **In** the past six months, the following companies have either attended DARG meetings or been given demonstrations of our real-time data acquisition system, flow injection analysis apparatus, absorbance-to-concentration and dyeing models, and control systems: Burlington Industries (several groups), American **&** Efird, National **Spinning,** Collins and Aikman, **Ciba,** and Jasper Textiles. Previous visitors have included Milliken, Russell, and Sara **Lee.**

At this time, we have made substantial **progress** toward each of the above goals, roughly indicated by the following. By the very nature of the above goals, some are logically accomplished before others, **therefore** progress toward goals varies.

	Long Term Goal	% Complete (or progress)
1.	Sensors (existing)	75%
2.	Sensors (new/develop)	40%
3.	Data handling	60%
4.	Control models	50%
5.	Dye models	50%
6.	Computing hardware	25%
7.	Human resources	2 M.S. students graduated under NTC 5 MS. students graduated under **NTC** + CRAFTM 1 **Ph.D** student graduated under NTC + **CRAFTM** 4 **Ph.D** students in project 2 open positions, one chemistry and one engineering

Technical Quality/Accomplishments:

As will be described in mote detail later, the DARG team is subdivided into **three** closely interacting groups: data acquisition, modeling, and **control.** Year two progress reported **here** is similarly divided.

Data Acquisition:

The flow injection analysis **(FIA)** system has been connected to a **Gaston** County laboratory-scale package machine at Ciba and calibrated with three-dye mixtures of Cibacton Red **C-2G,** Cibacron Navy C-B, and Cibacton Yellow C-R-01, in the range of 0.05 to 3.00 g/L. A multifile which shows all the data taken for a single calibration sample is shown in Figure 1. The system then was used to monitor the dyeing process for three different trichmmatic shade combinations. Information about the behavior of the three primary Cibacron C dyes during dyeing and their **final** exhaustion/fixation levels was obtained. The final dye concentrations, based on **FIA** measurements of dye concentration in the bath at the end of the dye cycle, were predicted by the Partial Least Squares **(PLS)** program, and were compared to color-matching predictions from reflectance **measurements** made on the dyed goods. There was good comparison between the **FIA-based** predictions and the reflectance-based concentration predictions. Testing of **various** models showed that absorbance measurements are linear in the 0 to 2 AU range. Based on the exhaustion curves, which **were** calculated for each component, the yellow dye has the highest initial exhaustion, and the navy dye has the highest **final** exhaustion. For hvo of the shades, all components exhausted in excess of 85%.

Two of the same shade combinations were repeated on a Texomat dye machine in the DARG laboratory and monitored with the **FIA** system to investigate possible noise in the sampling system and to verify the dyeing behavior which was shown in the package machine trials. The exhaustion curves for these dyeings were much smoother, which indicated that the package machine introduced a source of noise or error into the exhaustion curves for the package dyeings. Otherwise, the dyeing behavior was very similar to that obtained on the package machine. The exhaustion curves for the brown shade are shown in Figure 2.

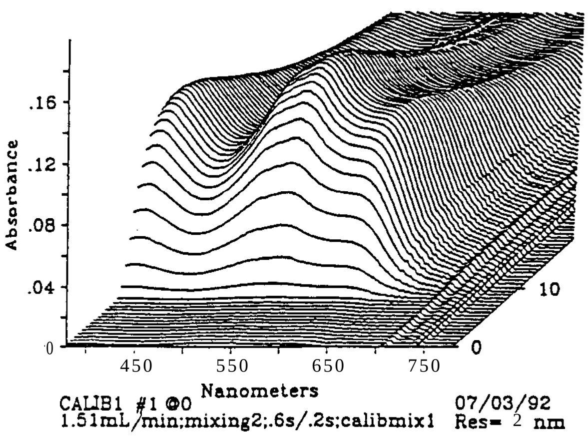

Figure 1. FIA **Multifile** of a Three-Dye Mixture

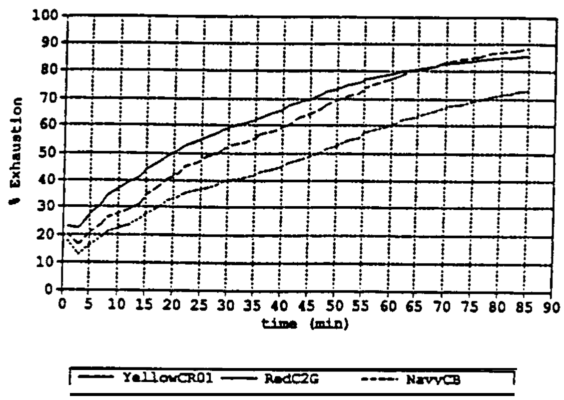

Figure 2. Exhaustion Curves for Brown Shade on Texomat

Other work has focused on finding a suitable commercial mixing chamber for dilution and a **continuous-**flow pump with equivalent precision. Initial results from experiments to determine concentration of disperse dyes by **FIA** look promising.

Several experiments have been conducted to determine the effects of dye concentration on aggregation and subsequent spectral shifts due to aggregation. Similar experiments have been used to determine the significance of interactions of dyes in mixtures, and the effects of auxiliaries on the spectra of individual dyes and dye mixtures. Figure 3 shows the effect of increasing concentrations of **NaCl** on the absorbance spectrum of Reactive Blue 52.

The modeling of **dyebath** mixtures using parametric and non-parametric models has resulted in the development of equations that predict the concentration of individual dyes **from** spectra of the mixtures of the dyes. Simple Beer's Law analysis has been compared to multiple regression and neural network analyses for comparison. Relationships regarding the effects of auxiliaries (such as salt and disaggregant) on the spectra of dyes and dye mixtures have been determined experimentally and are being quantified.

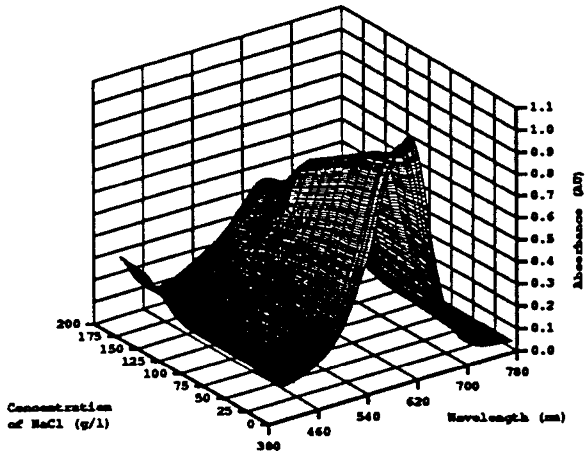

Figure 3. Effect of NaCl on Reactive Blue 52 Spectra

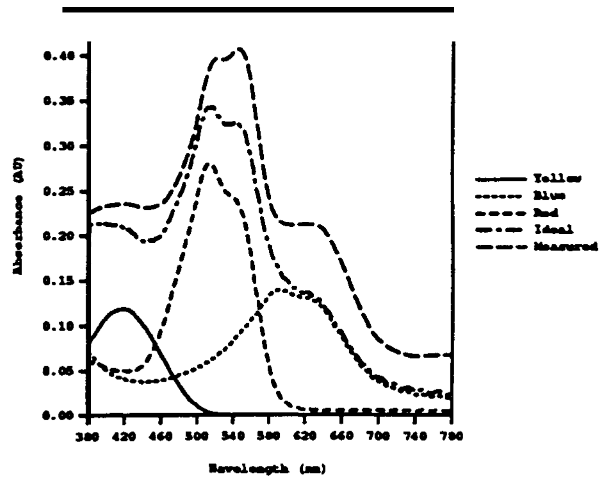

Figure 4. Spectra Illustrating Dye-Dye Interactions

Experiments on the nature of dye-dye interactions and the abiity (chemically and statistically) of two interacting dyes to interact with a third dye in a dyebath are being determined. Figure 4 shows the spectra of individual dyes (yellow, blue, and red), the “ideal” spectrum that is obtained by summing the individual spectral absorbances, and the actual spectrum of the dye mixture. The difference between the “ideal” and measured spectra is a function of interactions that are accounted for in our models for converting absorbance spectra to concentrations of individual dyes.

Since it is widely known that the intermolecular attraction of dyes and auxiliaries in dyebaths can affect the affinity of the dyes, experiments have been designed which will track the exhaustion of individual dyes in mixtures during the dyeing to see what effects dye aggregation and auxiliaries have on the kinetics of dye sorption. This knowledge should lead to a method of pre-testing dyes in mixtures to determine the compatibility of those dyes.

Modeling:

Development of theoretical models of the dyeing process continues to receive significant attention by our team. Dr. Ralph McGregor is currently on a scholarly assignment at the Swiss Federal Institute of Technology (ETH- Zurich) in Zurich, Switzerland. He is working in the research group of Professor Paul Rys on two major topics, one of which is the computer simulation of package dyeing. This work has been done by Professor Rys's group using a Cray 2 supercomputer at EPF-Lausanne, a Cray Y-MP at ETH-Zurich, and mote recently a NEC SX3/22 in Manno. In this work, the Navier-Stokes Equation has been solved for fluid flow in an assembly of fibers, together with the convective diffusion equations for the transport of dye to the fiber surfaces, and together also with the equations for diffusion and sorption of dye within the fibers.

It is now possible for any given time to calculate the instantaneous distribution of dye within the dye solution in the package, and within each **fiber.** Thus the effects of changes in the parameters which control the package-dyeing process can now be simulated at a level of detail not previously achieved to our knowledge. The possibility of continued collaboration in this area, through the North Carolina Computer Center, is being explored.

Modeling work was carried out in the DARG laboratory by applying dimensionless groups of variables, previously used for the description of sorption equilibria in ionic dyeing, to a system of a mixture of polysulfonated acid dyes on nylon. Data obtained **from** the literature **were** fitted to the model and very good least squares non-linear fits were obtained. **One** such least squares fit for the uptake of Acid Blue 45 on nylon is shown in Figure 5. This method may help to predict sorption isotherms without explicit calculation of the elusive electrical phenomena involved in the ionic equilibration The linkage of such equilibrium concepts with simplified kinetic equations is being explored as a means of both predicting and controlling the behavior of dyeing processes.

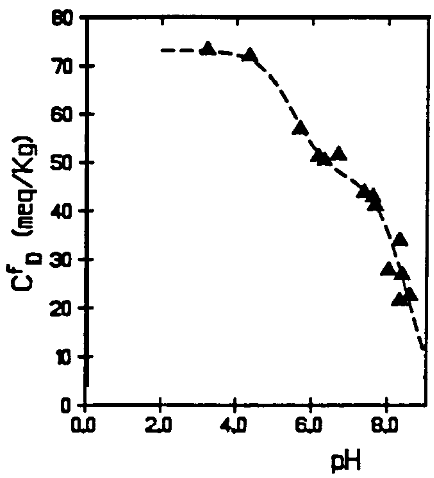

Figure 5. Actual (▲) and **Predicted** (-) Uptake of Acid Blue 45

Current DARG dyeing equipment has been modified to allow dosing of dyes and/or chemicals into the **dyebath** using a computer controlled peristaltic and/or piston pump. The software necessary to drive the pump was written and tested. The uptake of acid dyes by nylon will be controlled by dosing acid and/or dye(s) into the bath.

Controls:

A fuzzy logic controller, to assist the decision-making activities of an experienced dyer, has been developed to control dye concentration in batch dyeing processes. The control decisions of the dyer can be expressed linguistically as a set of heuristic decision **rules,** which **are** used to build rulebases for the controller. Also, certain algorithms are used to convert the rules to quantitative control outputs.

Based on previous work, we have tested enhanced fuzzy logic control schemes which can develop control rules automatically with very limited process knowledge, i.e. the controller has learning ability. Effort to combine fuzzy logic and optimization to control complex multi-input-multi-output(MIlvIO) system has

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been made. Computer simulations suggest that those schemes can control exhaustion of dyes in a multiple component **dyebath.** Through calibration measurements, a nonlinear mapping is empirically derived which relates absorbance spectra to dye concentration. The important control variables am the dye concentrations and the rate of change of the concentrations, both of which determine the levelness and shade of the fabric.

To enhance our abiity to monitor and control the batch dyeing process, a second data acquisition system was designed and implemented to monitor and control the dyeing process. The system design was predicated upon three ideas:

1. It should conform to public standards.
2. It should be modular for maximum flexibility
3. It should provide robust, **accurate,** and appropriate data collection

The final system consisted of a Motorola MVME 167 board running **VxWorks,** a real-time **POSIX** compliant operating system. The computer system incorporates the UNIX development environment with high-performance real-time hardware located near the dyeing apparatus. A network of **DECstations,** running ULTRIX 4.2, allows a window-based environment for pmgramming, debugging, analysis, and simulation. The real-time computer communicates with the network over **TCP/IP** to allow **programs** to be downloaded and experimental data to be uploaded to the server's **hard** disk With this system, dye exhaustion, **pH,** temperature, and conductivity can all be monitored in real-time.

Publications:

W. Jasper, E. Kovacs, and G. A. **Berkstresser,IV,** "Using Neural Networks to Predict Dye Concentrations in Multiple-Dye **Mixtures",** Textile Research Journal, (to appear September 1993).

J. Lu and G. Lee "A Self-Learning Fuzzy Logic Controller with On-line Scaling Factor Tuning", International Conference on Computer Applications, Long Beach CA (to appear March 1994).

G. A. Berkstresser IV, K. R. Beck, B. Smith, R. McGregor, and W. Jasper, "Novel Approaches for the Real-Time Prediction of Dye Concentrations in **Three** Dye Mixtures", Book of Papers, American Association of Textile Chemists and Colorists **International** Conference and Exhibition, Montreal, Quebec (to appear October 1993).

M. R. Lefeber, K. R. Beck, B. Smith, R McGregor, and W. Hunter, "Flow Injection Analysis of Dyebaths", Book of Papers, American Association of Textile Chemists and Colorists International Conference and Exhibition, Atlanta, GA, October 1992.

M. R. Lefeber, K. R. Beck, B. Smith, R. McGregor, and W. Hunter, "Flow Injection Analysis of Dyebaths", Textile Chemist and Colorist (accepted for publication).

R. McGregor and M. Arora. "Dimensionless Groups for the Sorption of Dye and other Ions by Polymers. III. Polysulfonated Acid Dyes and Polyamides", Submitted to Journal of Applied Polymer Science.

B. Smith and J. Lu, "Improving Computer **Control** of Batch Dyeing Operations", American **Dyestuff** Reporter (accepted for publication).

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E. T. Kovacs, "Utilization of Backpropagation Neural Networks to Interpret Spectral Data in Textiles: Two Applications", IMSEI Masters Thesis, NCSU, June 1993.

M. R. Lefeber, "Flow Injection Analysis of Dyebaths", TECS Masters Thesis, NCSU, July 1993.

Presentations:

G. A. Berkstresser IV, K.R. Beck, C.B. Smith, W.J. Jasper, and R. McGregor, "On-Line Continuous Determination Of Individual Dye Concentrations From Spectra Of Dye Mixtures In Solution: Deviations From Beer's Law, American Chemical Society North Carolina Sectional Meeting, Raleigh NC, April 1993.

K. R. Beck, M. Arora, G. A. Berkstresser, IV, W. Jasper, G. Lee, M. R Lefeber, J. Lu, R. McGregor, and B. Smith, "Real-Tie Data Acquisition, Theoretical Modeling, and Adaptive Control of Batch Dyeing Process", Institute for Textile Technology Technical Advisory Committee Meeting Invited Paper, April 1993.

K. R Beck, M. Arora, G. A. Berkstresser, IV, W. Jasper, G. Koksal, M. R. Lefeber, J. Lu, R McGregor, B. Smith, and W. Smith, "Real-Tie Data Acquisition, Theoretical Modeling, and Adaptive Control of Batch Dyeing Processs", First Annual National Textile Center Forum Plenary Session, Auburn, AL, February 1993.

M. R. Lefeber, K. R. Beck, B. Smith, R McGregor, and W. Hunter, "Flow Injection Analysis of Dyebaths", American Association of Textile Chemists and Colorists International Conference and Exhibition, Atlanta, GA, October 1992.

Resource Management:

Three chemists and two mechanical/aerospace engineers, three Fiber and Polymer Science Ph.D. students and one Mechanical Engineering Ph.D student currently comprise the Dye Applications Research Group. A Mechanical Engineering MS. student specializing in controls has been recruited. A fourth textile chemistry student is being recruited for January 1994. To compliment the knowledge of the DARG members, Dr. Bill Hunter, an analytical chemist from Ciba has joined the group and has been instrumental in FIA development and other chemistry related portions of the project. Overall, the group remains completely focused on the goal of adaptively controlling the batch dyeing process through teal-time data acquisition, theoretical modeling, and innovative control strategies.

All students are housed in same modem office/lab complex. This promotes facile generation and exchange of information Electronic-mail is used on a daily basis to communicate among members of the group. Meeting schedules and agendas, research ideas and suggestions, manuscripts for publication, and requests for report materials are some of the types of information passed electronically. Because the DARG complex is connected to the College of Textiles network, students and faculty have access to word processors, an engineering spreadsheet, symbolic math, SAS, and programming languages. All of these tools are utilized in our research effon In bi-weekly meetings, general project information is shared with group members and students present and defend their work. Typically, one student has responsibility for a detailed presentation and others present summaries. Numerous groups that have attended meetings or demonstrations have been most complimentary about both the quality of the students in the

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project and the significance of their work. Summaries of our research progress are displayed on bulletin boards inside and outside the DARG lab and are available for viewing by casual observers and as visual aids to explain the goals and integrated nature of the project to visitors.

To promote the exchange of information between the group members and industry, field trips to Burlington Industries Wake Finishing Plant and National Spinning have been taken.

DARG research goals and results were featured in a SEARCH program on PBS in August 1993.

In addition to providing financial support for project personnel, NTC funds have been used to purchase a low liquor ratio single-package dyeing machine that will allow development of a second data acquisition system. Year one funds were used to develop the FIA system that will now be interfaced with the new dyeing machine when it is delivered (Manufacturing problems have caused a six-month delay in delivery.). ***Year two*** funds are also being used to replace the aging VMS VAX based data acquisition hardware with an in-house developed Unix based system with greatly enhanced capabilities and reduced maintenance costs. The original VAX system cost nearly $80,000 while the new system will cost less than $15,000. Year two funds are also being used to purchase multiplexing equipment so that multiple dyeings can be monitored and controlled simultaneously.

Conclusions:

The following are major year-two contributions by the Dye Applications Research Group:

Data Acquisition

1. Flow injection analysis has been further developed and implemented on both a laboratory dyeing and a pilot scale package dyeing machine. Using FIA it has been possible to determine exhaustion characteristics of individual fiber reactive dyes.
2. Sophisticated calibration models that account for dye-dye and salt-dye interactions have been developed. Both non-linear neural network models and linear regression models have proven to accurately predict individual dye concentrations.

Theoretical Modeling

1. Using dimensionless groups to simplify complex interactions, a theoretical model that accurately predicts uptake of acid dyes has been developed.
2. Capability for computer-controlled dosing of acid, alkali, salt, and dyes has been developed.

Controls:

1. A novel self-tuning fuzzy logic controller that can automatically develop control rules has been developed.
2. A second flexible and powerful data acquisition/control system based on standards and in-house software has been assembled and tested.

Our efforts to transfer this information to industry have generated considerable interest. We plan to pursue further technology transfer activities.