GEORGIA INSTITUTE OF TECHNOLOGY — OFFICE OF CONTRACT ADMINISTRATION

PROJECT ADMINISTRATION DATA SHEET

[x] ORIGINAL [ ] REVISION NO. _____

Project No. E-19-608 GTRI/~~GIT~~ DATE 11/2/82

Project Director: F. Joseph Schork School/~~Lab~~ ChE

Sponsor: American Chemical Society

Type Agreement: Grant In Aid PRF #14149 GF

Award Period: From 10/1/82 To ~~8/31/84~~ 8-31-85 (Performance) 8/31/84 (Reports)

Sponsor Amount: Total Estimated: $ 10,000 Funded: $ 10,000

Cost Sharing Amount: $ _____ Cost Sharing No: _____

Title: Optimal Control of Batch Emulsion Polymerization Reactors

ADMINISTRATIVE DATA

OCA Contact Linda H. Bowman

1) Sponsor Technical Contact:

Dr. Joseph E. Rogers, Jr.
The Petroleum Research Fund
American Chemical Society
1155 16th St. NW
Washington, DC 20036

2) Sponsor Admin/Contractual Matters:

Defense Priority Rating: none

Military Security Classification: none
(or) Company/Industrial Proprietary: _____

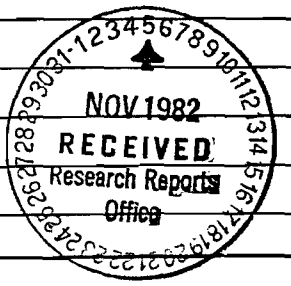
RESTRICTIONS

See Attached na Supplemental Information Sheet for Additional Requirements.

Travel: Foreign travel must have prior approval – Contact OCA in each case. Domestic travel requires sponsor approval where total will exceed greater of $500 or 125% of approved proposal budget category.

Equipment: Title vests with GIT

COMMENTS:



COPIES TO:

Research Administrative Network	Research Security Services	Research Communications (2)
Research Property Management	Reports Coordinator (OCA)	Project File
Accounting	GTRI	Other _____
Procurement/EES Supply Services	Library	Other _____

FORM OCA 4:781 (Rev 982)

GEORGIA INSTITUTE OF TECHNOLOGY OFFICE OF CONTRACT ADMINISTRATION

SPONSORED PROJECT TERMINATION/CLOSEOUT SHEET

Date March 4, 1986

Project No. E-19-608 School/~~XXX~~ ChE

Includes Subproject No.(s) N/A

Project Director(s) F. Joseph Schork GTRI

Sponsor American Chemical Society

Title Optimal Control of Batch Emulsion Polymerization Reactors

Effective Completion Date: 8/31/85 (Performance) (Reports)

Grant/Contract Closeout Actions Remaining:

- [X] None
- [ ] Final Invoice or Final Fiscal Report
- [ ] Closing Documents
- [ ] Final Report of Inventions
- [ ] Govt. Property Inventory & Related Certificate
- [ ] Classified Material Certificate
- [ ] Other

Continues Project No. Continued by Project No.

COPIES TO:

Project Director
Research Administrative Network
Research Property Management
Accounting
Procurement/GTRI Supply Services
Research Security Services
[redacted]
Legal Services

Library
GTRC
Research Communications (2)
Project File
Other Heyser, Jones, Embry

FORM OCA 69.285

PERSONNEL STATEMENT

PRF# 14 149-G7 REPORTING PERIOD 9/1/82 TO 8/31/83

GRANTEE INSTITUTION Georgia Institute of Technology DEPARTMENT School of Chemical Engineering

PRINCIPAL INVESTIGATOR(S) Dr. F. Joseph Schork

GRANT PROJECT TITLE "Optimal Control of Batch Emulsion Polymerization Reactors"

List undergraduate, graduate, and postdoctoral co-workers receiving stipends under the above named grant:

NAME	TITLE OR ACADEMIC APPOINTMENT	PREVIOUS EDUCATION & DEGREES*	COUNTRY OF PERMANENT RESIDENCE	PERIOD OF SUPPORT (MONTHS)	PERCENT OF SUPPORT FROM PRF **	DEGREES RECEIVED (IF ANY) DURING REPORTING PERIOD
None						

List other co-workers on grant project not directly supported with ACS - PRF funds:

NAME	SOURCE OF SUPPORT	DATES ASSOCIATED WITH GRANT PROJECT
Mark Perri	Chevron Fellowship	October, 1982 - Present

* For graduate students, indicate the College or University attended prior to graduate work. For postdoctoral fellows, give the name of the Ph. D. granting institution.

** (... the period stated in preceding column)

THE PETROLEUM RESEARCH FUND

REPORT ON ACTIVITY ASSISTED BY

GRANT, PRF # 14149-G7

Page ____ of ____ pages.

PREPARED BY

F. Joseph Schork

Date October 4, 1983

Please refer to instructions.

Fill in information requested above for each page.

The report heading, narrative, and all drawings must be prepared within the box.

Please submit one sharp, clear "original" and a copy (Xerox, carbon, etc.) for each page.

14149-G7 Optimal Control of Batch Emulsion Polymerization Reactors

F. Joseph Schork, Georgia Institute of Technology

A dynamic mathematical model of the batch emulsion polymerization process has been developed and is currently being tested to evaluate its ability to adequately simulate experimental results on the batch emulsion polymerization of methyl methacrylate stabilized with sodium lauryl sulfate and initiated with ammonium persulfate. Preliminary results are encouraging.

The model consists of a set of ordinary differential equations involving balances over initiator concentration, polymer concentration and particle number. Monomer conversion and average particle volume are calculated algebraically from the above. Surfactant concentration is assumed to remain in equilibrium, and hence the number of micelles can be calculated from a steady-state surfactant balance. Particle initiation is assumed to take place via the classical micellar initiation mechanism. A modification of the Flory-Huggins Equation is used to calculate the degree of particle swelling with monomer. A modification of the gel effect correlation of Hamielec and coworkers (1) is employed.

It is anticipated that the modeling work will be completed shortly. Work will then begin on the development of a linear quadratic optimal controller for this system. Controller performance will be evaluated by simulation employing the mathematical model recently developed.

(1) Friis, N., Hamielec, A. E., Polymer Preprints, p. 192, ACS Meeting, 1975.

PERSONNEL STATEMENT

PRF# 14149-G7 REPORTING PERIOD Sept. 1, 1983 TO August 31, 1984

GRANTEE INSTITUTION Georgia Institute of Technology DEPARTMENT Chemical Engineering

PRINCIPAL INVESTIGATOR(S) F. Joseph Schork

GRANT PROJECT TITLE Optimal Control of Batch Emulsion Polymerization Reactors

List undergraduate, graduate, and postdoctoral co-workers receiving stipends under the above named grant:

NAME	TITLE OR ACADEMIC APPOINTMENT	PREVIOUS EDUCATION & DEGREES*	COUNTRY OF PERMANENT RESIDENCE	PERIOD OF SUPPORT (MONTHS)	PERCENT OF SUPPORT FROM PRF **	DEGREES RECEIVED (IF ANY) DURING REPORTING PERIOD
F. J. Schork	Asst. Prof.	PhD	USA	2	34%	--
M. J. Perri	Res. Asst.	BS	USA	3	50%	--
H. C. Lee	Res. Asst.	MS	Taiwan	3	25%	--

List other co-workers on grant project not directly supported with ACS - PRF funds:

NAME	SOURCE OF SUPPORT	DATES ASSOCIATED WITH GRANT PROJECT
None		

* For graduate students, indicate the College or University attended prior to graduate work. For postdoctoral fellows, give the name of the Ph. D. granting institution.

** (during the period stated in preceding column)

Revised 6/82

THE PETROLEUM RESEARCH FUND

REPORT ON ACTIVITY ASSISTED BY

GRANT, PRF # 14149-G7

Page 1 of 2 pages.

PREPARED BY

F. Joseph Schork

Date September 11, 1984

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Fill in information requested above for each page.

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14149-G7 Optimal Control of Batch Emulsion Polymerization Reactors

F. Joseph Schork, Georgia Institute of Technology

A dynamic model of the batch emulsion polymerization process has been developed. Comparison with laboratory data indicates that the model is capable of adequately describing the batch emulsion polymerization of methyl methacrylate.

The model consists of a set of ordinary differential equations representing mass balances over initiator concentration, polymer concentration, and particle number. Monomer conversion and average particle volume are calculated algebraicly from the above. Equilibrium particle swelling is assumed, and is calculated according to Morton (1). Gel effects for termination and propagation are incorporated after Jaisinghani (2) and Ross (3), respectively.

Due to the nature of the emulsion polymerization process, the model is highly nonlinear. For a batch process, linearization is not appropriate. It has been decided, therefore, to treat the optimal control of batch emulsion polymerization as a multidimensional nonlinear optimization problem for which the solution is the open-loop control policy by which initiator and surfactant will be introduced into the reactor during polymerization in order to minimize some objective function involving cost and product quality considerations. The optimization is additionally constrained by the heat-removal capability of the reactor. Current commercial practice involves the application of empirical open-loop policies. This work will develop such policies directly from a knowledge of the mechnism of polymerization.

The optimization is greatly complicated by the existence of mathematical discontinuities in the model at the transitions from Interval I to Interval II, and from Interval II to Interval III. Computational techniques for optimization of systems containing discontinuities are not well developed (4). Currently six computational techniques are being evaluated. From these

THE PETROLEUM RESEARCH FUND

REPORT ON ACTIVITY ASSISTED BY

GRANT, PRF # 14149-G7

PREPARED BY

F. Joseph Schork

Date September 11, 1984

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two techniques will be selected and applied to the problem at hand.

(1) Morton, M., Kaizerman, S, and Altier, M., J. Colloid Sci. (1954) 9, 300.

(2) Jaisinghani, R., and Ray, W., Chem. Eng. Sci. (1977) 32, 811.

(3) Ross, R., and Laurence, R., AIChE Symp. Ser. (1976) 72, 74.

(4) Bryson, A., and Ho, Y., Applied Optimal Control (1975) Wiley, N.Y.