GEORGIA INSTITUTE OF TECHNOLOGY — OFFICE OF CONTRACT ADMINISTRATION

PROJECT ADMINISTRATION DATA SHEET

[X] ORIGINAL [ ] REVISION NO. ______

Project No./(Center No.) E-19-652 (R6304-0A0) GTRC/XXX DATE 5 / 8 / 87

Project Director: A. H. Skelland School/XXX Ch E

Sponsor: National Science Foundation

Agreement No.: Grant No. CBT-8603984

Award Period: From 4/1/87 To 9/30/88 * (Performance) 12/30/88 Reports

Sponsor Amount:

	New With This Change	Total to Date
Contract Value:	$	$ 58,849
Funded:	$	$ 58,849

Cost Sharing No./(Center No.) E-19-342 (F6304-0A0) Cost Sharing: $ 1189

Title: Continuation of Studies on Dispersion and Mass Transfer in Agitated Liquid - Liquid Systems.

ADMINISTRATIVE DATA

OCA Contact John B. Schonk X-4820

1) Sponsor Technical Contact:

Raj Rajagopalan
National Science Foundation
ENG/CBT
Washington, D.C. 20550
202/357-9606

2) Sponsor Issuing Office:

Mary Frances
National Science Foundation
DGC/ENG
Washington, D.C. 20550
202/357-9626

Military Security Classification: ______
(or) Company/Industrial Proprietary: ______

ONR Resident Rep. is ACO: ______ Yes ______ No
Defense Priority Rating: ______

RESTRICTIONS

See Attached NSF 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:

*No funds may be expended after 9/30/88.

COPIES TO:

SPONSOR'S I.D. NO. ______

Project Director	Procurement/GTRI Supply Services	GTRC
Research Administrative Network	Research Security Services	Library
Research Property Management	Contract Support Div.(OCA)(2)	Project File
Accounting	Research Communications	Other

GEORGIA INSTITUTE OF TECHNOLOGY
OFFICE OF CONTRACT ADMINISTRATION

NOTICE OF PROJECT CLOSEOUT

Closeout Notice Date 01/23/91

Project No. E-19-652 | Center No. R6304-0A0

Project Director SKELLAND A H | School/Lab CHEM ENGR

Sponsor NATL SCIENCE FOUNDATION/GENERAL

Contract/Grant No. CBT-8603984 | Contract Entity GTRC

Prime Contract No.

Title STUDIES ON DISPERSION AND MASS TRANSFER IN AGITATED LIQUID-LIQUID SYSTEMS

Effective Completion Date 880930 (Performance) 881231 (Reports)

Closeout Actions Required:	Y/N	Date Submitted
Final Invoice or Copy of Final Invoice	Y	
Final Report of Inventions and/or Subcontracts	Y	910107
Government Property Inventory & Related Certificate	N	
Classified Material Certificate	N	
Release and Assignment	N	
Other	N	

Comments

Subproject Under Main Project No.

Continues Project No.

Distribution Required:

Project Director	Y
Administrative Network Representative	Y
GTRI Accounting/Grants and Contracts	Y
Procurement/Supply Services	Y
Research Property Managment	Y
Research Security Services	N
Reports Coordinator (OCA)	Y
GTRC	Y
Project File	Y
Other	N
	N

NOTE: Final Patent Questionnaire sent to PDPI.

E-19-652

NATIONAL SCIENCE FOUNDATION
Washington, D.C. 20550

FINAL PROJECT REPORT
NSF FORM 98A

PLEASE READ INSTRUCTIONS ON REVERSE BEFORE COMPLETING

PART I—PROJECT IDENTIFICATION INFORMATION

1. Institution and Address	2. NSF Program	3. NSF Award Number
Georgia Institute of Technology Atlanta, GA 30332	Separation & Purification	CBT-8603984
	4. Award Period From 3/1/87 To 6/1/88	5. Cumulative Award Amount $58,849

6. Project Title
Continued Study of Dispersion and Mass Transfer in Agitated Liquid-Liquid Systems.

PART II—SUMMARY OF COMPLETED PROJECT *(FOR PUBLIC USE)*

This grant partially supported work which was a continuation of that performed with NSF support by grants CPE-8203872 and CPE-8203872/01, as described in the final report on those grants, submitted at an earlier date. It also provided partial support for the Principal Investigator during subsequent preparation of the papers published on the basis of that work. (See publication citations 1-8).

The continuation work culminated in the Ph.D. thesis by Dr. Jeffrey S. Kanel in 1990, entitled "Effects of Some Interfacial Phenomena on Mass Transfer in Agitated Liquid-Liquid Dispersions." This study developed analytical relationships for mass transfer during drop breakage, during binary drop coalescence, and during binary drop collision and rebounding. These expressions were combined with mass transfer rates from drops moving around the baffled vessel between each of these events, along with equations for drop breakage and coalescence frequencies and a population balance, to predict total transfer as a function of time in batch operation.

These predictions compared well with measurements of drop size and total transfer as each run progressed. Experimental variables included the direction of mass transfer, the selection of the disperse phase, the concentration of a nonionic surfactant, the volume fraction of disperse phase, and the speed and size of impeller, in a factorially designed program of 256 runs.

Eight papers from the work are in various stages of publication, as noted in Part III and citations 9-16.

PART III—TECHNICAL INFORMATION *(FOR PROGRAM MANAGEMENT USES)*

1. ITEM *(Check appropriate blocks)*	NONE	ATTACHED	PREVIOUSLY FURNISHED	TO BE FURNISHED SEPARATELY TO PROGRAM: Check (✓)	Approx. Date
a. Abstracts of Theses		✓			
b. Publication Citations		✓			
c. Data on Scientific Collaborators					
d. Information on Inventions					
e. Technical Description of Project and Results					
f. Other *(specify)*					

2. Principal Investigator/Project Director Name *(Typed)*	3. Principal Investigator/Project Director Signature	4. Date
A. H. P. SKELLAND		Jan 3, 1991

NSF Form 98A (1-87) Supersedes All Previous Editions

Form Approved OMB No. 3145-0058

PART IV - SUMMARY DATA ON PROJECT PERSONNEL

NSF Division ______________________

The data requested below will be used to develop a statistical profile on the personnel supported through NSF grants. The information on this part is solicited under the authority of the National Science Foundation Act of 1950, as amended. All information provided will be treated as confidential and will be safeguarded in accordance with the provisions of the Privacy Act of 1974. NSF requires that a single copy of this part be submitted with each Final Project Report (NSF Form 98A); however, submission of the requested information is not mandatory and is not a precondition of future awards. If you do not wish to submit this information, please check this box ☐

Please enter the numbers of individuals supported under this NSF grant.
Do not enter information for individuals working less than 40 hours in any calendar year.

*U.S. Citizens/ Permanent Visa	PI's/PD's		Post-doctorals		Graduate Students		Under-graduates		Precollege Teachers		Others	
	Male	Fem.	Male	Fem.	Male	Fem.	Male	Fem.	Male	Fem.	Male	Fem.
American Indian or Alaskan Native												
Asian or Pacific Islander												
Black, Not of Hispanic Origin												
Hispanic												
White, Not of Hispanic Origin	√(1)				1							
Total U.S. Citizens					1							
Non U.S. Citizens	1											
Total U.S. & Non-U.S. ..	1				1							
Number of individuals who have a handicap that limits a major life activity.												

*Use the category that best describes person's ethnic/racial status. (If more than one category applies, use the one category that most closely reflects the person's recognition in the community.)

AMERICAN INDIAN OR ALASKAN NATIVE: A person having origins in any of the original peoples of North America, and who maintains cultural identification through tribal affiliation or community recognition.

ASIAN OR PACIFIC ISLANDER: A person having origins in any of the original peoples of the Far East, Southeast Asia, the Indian subcontinent, or the Pacific Islands. This area includes, for example, China, India, Japan, Korea, the Philippine Islands and Samoa.

BLACK, NOT OF HISPANIC ORIGIN: A person having origins in any of the black racial groups of Africa.

HISPANIC: A person of Mexican, Puerto Rican, Cuban, Central or South American or other Spanish culture or origin, regardless of race.

WHITE, NOT OF HISPANIC ORIGIN: A person having origins in any of the original peoples of Europe, North Africa or the Middle East.

THIS PART WILL BE PHYSICALLY SEPARATED FROM THE FINAL PROJECT REPORT AND USED AS A COMPUTER SOURCE DOCUMENT. DO NOT DUPLICATE IT ON THE REVERSE OF ANY OTHER PART OF THE FINAL REPORT.

EFFECTS OF SOME INTERFACIAL PHENOMENA ON MASS TRANSFER IN AGITATED LIQUID-LIQUID DISPERSIONS

A THESIS

Presented to
the Faculty of the Division of Graduate Studies
The Georgia Institute of Technology
By
Jeffrey Scott Kanel

In Partial Fulfillment
of the Requirements for the Degree of
Doctor of Philosophy in Chemical Engineering
March 19, 1990

EFFECTS OF SOME INTERFACIAL PHENOMENA ON MASS TRANSFER IN AGITATED LIQUID-LIQUID SYSTEMS

Approved:

A.H. Peter Skelland, Chairman

Larry J. Forney

Charles L. Liotta

Michael J. Matteson

Ronald W. Rousseau

Date approved by Chairman 4/3/90

ABSTRACT

The chemical process industry utilizes many operations, such as liquid-liquid extraction and multiphase reactors, that rely upon a solute transferring between two immiscible liquids. In these systems mass transfer occurs during the phenomena of drop breakup, free movement of the drops throughout the vessel, drop oscillations, and drop-drop collisions resulting in either coalescence or rebounding. Thus, the objectives of this study were first to develop models for interfacial mass transfer during each of these processes. These models were used to derive expressions for the individual dispersed and continuous phase mass transfer coefficients for each event. Subsequently, these expressions were assembled into a simulation routine that predicted the rate of mass transfer and the transient Sauter-mean drop diameter in batch agitated dispersions. Using sixteen different expressions, eight of which were developed in this study, the transient fractional mass transfer was felt to be well predicted with a ± 20% average deviation for all four combinations of the directions of diffusion and dispersion, when no adjustable parameters were used. However, to further enhance the simulation, one constant in the breakage frequency was varied that improved predictions to ± 15% for 10 simulations, regardless of the directions of diffusion and dispersion or surfactant concentration. Furthermore, the transient Sauter-mean drop diameter was predicted with a ± 8% average deviation for these simulations.

The second objective was to determine the effect of reversing both the direction of diffusion and dispersion on the rate of solute transfer in order to elucidate one or more optimal contacting schemes for design purposes. Variations in the solute transfer rate for these four permutations could have resulted from Marangoni instability or hydrogen bonding between the solute and the solvent that initially contained it. Coalescence frequencies also depend on the transfer direction, and this constituted an

additional modification. The third objective was to determine the effect of surfactant concentration on the rate of mass transfer, since surfactants are frequently encountered as contaminants in liquid-liquid extractors. Compounds that behave surface actively are also secreted by cells in fermentors while surfactants are purposely added in emulsion polymerizers.

The second and third objectives were examined with a full factorial analysis experimental design with the following variables: four surfactant (Triton X-100) concentrations (one with no surfactant; one that produced a minimal interfacial tension, and two intermediate concentrations), two impeller diameters (0.1015 and 0.0631 m); two volume fractions of the dispersed phase (0.07 and 0.03); four impeller speeds (above the minimum impeller speed for complete dispersion); and both directions of diffusion and dispersion. Water and chlorobenzene were the solvents with tetrabutylammonium bromide, TBAB, transferring across the interface. A cylindrical vessel (diameter of 0.2135m), filled to a height equal to its diameter, with four 8.9% baffles was used in conjunction with a centrally mounted six flat-blade turbine impeller. Photographs of the dispersion were used to obtain the interfacial area so that area - free mass transfer coefficients, K, could be obtained.

When the direction of dispersion and diffusion were varied, several observations were made. First, the mass transfer coefficient was enhanced with diffusion from chlorobenzene drops at low surfactant concentrations, [SAA]. However, K was not increased in this case at high [SAA]. Second, transfer of TBAB from the continuous chlorobenzene phase was slightly greater, on average, than that with diffusion in the opposite direction at low [SAA]. But, at the two highest surfactant concentrations, the direction of mass transfer when water was dispersed did not influence K.

When the [SAA] was varied, two different results were obtained that depended upon which solvent initially contained the TBAB. With solute transfer from chlorobenzene, the mass transfer coefficient decreased rapidly for [SAA] $\leq$ 0.1g/l water. However, at higher concentrations, it either reached a constant value or was slightly enhanced. When TBAB transferred from the aqueous phase, increasing surfactant concentrations resulted in augmented mass transfer coefficients.

Publications that are partially attributable to support from NSF Grant No. CBT-8603984

1. "Minimum Agitator Speed for Complete Liquid-Liquid Dispersion," by A. H. P. Skelland and G. G. Ramsay, Industrial and Engineering Chemistry Research, 26, 77-81, (1987).

2. "Effects of Surface Active Agents on Drop Size, Terminal Velocity, and Droplet Oscillation in Liquid-Liquid Systems," by A. H. P. Skelland, S. Woo, and G. G. Ramsay, Industrial and Engineering Chemistry Research, 26, 907-911, (1987)

3. "Effects of Surface Active Agents on Minimum Impeller Speeds for Liquid-Liquid Dispersion in Baffled Vessels," by A. H. P. Skelland and L. T. Moeti, Industrial and Engineering Chemistry Research, 28, 122-127, (1989).

4. "The Effects of Surface Active Agents on Jet Breakup in Liquid-Liquid Systems," by A. H. P. Skelland and P. G. Walker, The Canadian Journal of Chemical Engineering, 67, 762-770, (1989).

5. "Disperse-Phase Mass Transfer in Agitated Liquid-Liquid Systems," by A. H. P. Skelland and Hu Xien, Industrial and Engineering Chemistry Research, 29, 415-420, (1990).

6. "Effects of Surface Active Agents on Drop Size in Liquid-Liquid Systems" A. H.P. Skelland and E. A. Slaymaker, Industrial and Engineering Chemistry Research, 29, 494-499, (1990).

7. "Minimum Impeller Speeds for Complete Dispersion of Non-Newtonian Liquid-Liquid Systems in Baffled Vessels," by A. H. P. Skelland and J. S. Kanel, Industrial and Engineering Chemistry Research, 29, 1300-1306, (1990).

8. "Mechanism of Continuous Phase Mass Transfer in Agitated Liquid-Liquid Systems," by A. H. P. Skelland and L. T. Moeti, Industrial and Engineering Chemistry Research, 29, 2258-2267, (1990).

9. "Simulation of Mass Transfer in a Batch Agitated Liquid-Liquid Dispersion", by A. H. P. Skelland and J. S. Kanel, accepted for publication - subject to minor revision - in Industrial and Engineering Chemistry Research.

10. "Transient Drop Size in Agitated Liquid-Liquid Systems, as Influenced by the Direction of Mass Transfer and Surfactant Concentration", by A. H. P. Skelland and J. S. Kanel, accepted for publication - subject to minor revision - in Industrial and Engineering Chemistry Research.

11. "Transfer Direction, Disperse-Phase Selection, and Surfactants Influence Extraction in Agitated Liquid-Liquid Systems", by A. H. P. Skelland and J. S. Kanel, accepted for publication - subject to minor revision - in Industrial and Engineering Chemistry Research.

12. "Continuous Monitoring of Mass Transfer Rates in Batch Agitated Liquid-Liquid Systems by Electrical Conductivity", by A. H. P. Skelland and J. S. Kanel, accepted for publication - subject to minor revision - in Chemical Engineering Communications.

13. "Drop Breakage in Agitated Liquid-Liquid Systems Undergoing Mass Transfer", by A. H. P. Skelland and J. S. Kanel, in the course of publication.

14. "Mass Transfer during Drop-Drop Interactions", by A. H. P. Skelland and J. S. Kanel, in the course of publication.

15. "Mass Transfer during Drop Breakup and Subsequent Damped Oscillations in a Turbulent Field", by A. H. P. Skelland and J. S. Kanel, in the course of publication.

16. "Effects of Mass Transfer and Surfactants on the Minimum Impeller Speed for Complete Dispersion in Liquid-Liquid Systems", by A. H. P. Skelland and J. S. Kanel, in the course of publication.