Process Simulation in the 1960s and 1970s

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Summer 1965 10-Week Workshop – Computers in Engineering Design Education

40 Faculty – 5 fields
Ann Arbor, MI

PACER – Process Assembly Case Evaluator Routine

– Paul T. Shannon

Dartmouth College

Steady-State Chemical Process Simulation
Process Unit Subroutines
Sequential-Modular Approach
No Physical Property System

Batch Processing, Punched Cards, Printed Output

Time-Sharing – GE 235 Computer
- Interactive teletypewriter – phone lines

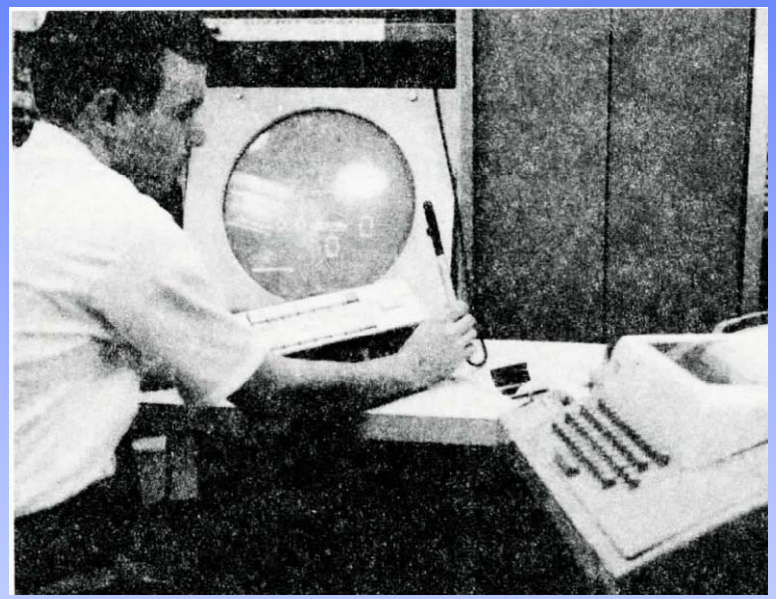
Time-Shared PACER – Dan Frantz
Univ. Michigan

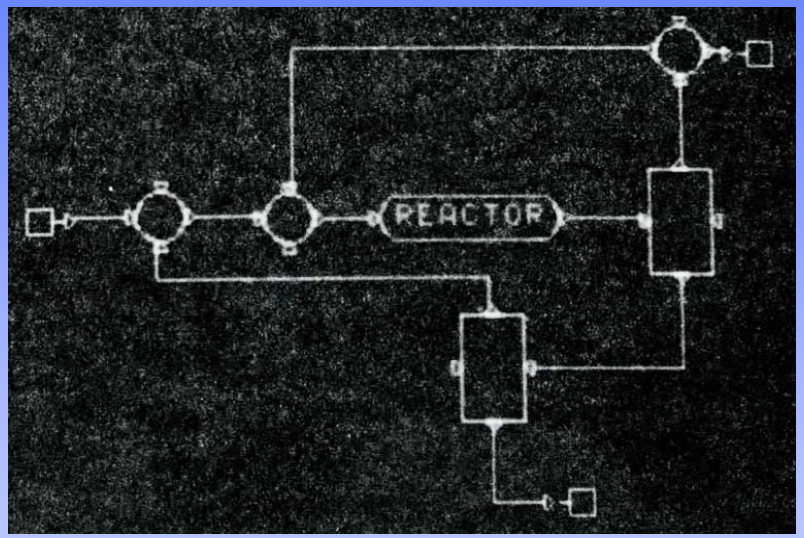
Entered flowsheet connectivity, feed stream and equipment parameter specifications, …

Provided results immediately! Made changes – re-ran

Time-Shared RCA Spectra 70/46 + DEC 338 Cathode Ray Tube Terminal ($100K)

Drew chemical process flowsheet using light-pen





Super-8 film demo.

New Orleans AIChE

March 1969

AIChE Machine Computation Committee

Created the AIChE Physical Property Estimation System in the late 1960s

Sought to select the best estimation path by minimizing cumulative error estimates

CHESS - Chemical Engineering Simulation System - 1968

Rudolphe L. Motard
Ernest J. Henley
Univ. of Houston

Steady-State Simulator
Sequential-Modular Approach
VLE Thermophysical Property Estimation

Evans, L. B., D.G. Steward, and C. R. Sprague, Computer-Aided Chemical Process Design, *Chem. Eng. Prog.*, 64 (4), 39-46, April 1968.

A comprehensive review of the state-of-the-art and projection of the great potential for computer-aided chemical process design

CHEOPS (Shell), Flexible Flowsheets (Kellogg), Chevron System

Frameworks – Data Structures, Matrix Structures

Physical Property Estimation (R. C. Reid)

Solution Algorithms

Several Research Projects

Translate FORTRAN programs that model process units into PACER subroutines – Penn

Create equation-oriented process simulators

SPEEDUP – Imperial College

ASAP – OLI Corporation

Create sequential-modular dynamic process simulator

DYNSYS – Western Ontario

REMUS - Penn

CACHE – Computer Aids for Chemical Engineering Education

Numerous incentives for inter-university cooperation, including

- potential for sharing in program and database development – beyond PACER, CHESS

- existence of the COSINE Committee – in Comp. Sci & E.E.

  - similar NSF startup funding recommended with coordination by the Commission on Education of the National Academy of Engineering

Initial focus of CACHE - 1969

15 founding members were using "modern" computers

- in research and teaching, creating:

  equation solvers
  process simulators
  databases
  physical property systems

- challenged by small, slow computers – with limited access, early programming languages.

CACHE Meeting – Boar's Head Inn – Charlottesville, VA Nov. 1974

Large-Scale Systems Task Force – chair, J. D. Seader

Initially, expected to create a more advanced simulator for use at universities

Instead, convinced Monsanto Corp. to make their pioneering process simulator, FLOWTRAN, available for use at universities over the United Computing Systems network

We wrote:

Seader, J.D., W.D. Seider, and A.C. Pauls, FLOWTRAN Simulation – An Introduction, CACHE, 1974

- placed emphasis on the advanced program architecture – permitting users to prepare customized simulation algorithms

- Third Edition in 1987

As university computers were connected with the ARPANET, working with EDUCOM, CACHE sought to install FLOWTRAN on a single university computer – for access across U.S.

When mini-computers became available to ChE Departments in the 1980s, Bob prepared load modules for installation of FLOWTRAN on over 180 departmental computers worldwide.

FLOWTRAN continued to be used at universities until the early 1990s when PC GUIs became available for the major process simulators (ASPEN PLUS, HYSYS, PRO/II, CHEMCAD, etc.)

CACHE Finances –

NSF - 1971-1975 (2-year projects)

Non-Profit CACHE Corp. (Massachusetts)

Larry Evans – handled incorporation
wrote the CACHE Bylaws
first CACHE Executive Officer
first CACHE News Editor

- an initial indication of his excellent organizational and managerial skills

Sabbatical – 1974-75 Academic Year

Cambridge (England or Massachusetts?)

University of Cambridge – CAD Center
Art Westerberg, Rudy Motard
Process Flowsheeting

M.I.T. – with Larry
"Developing modern CAD techniques related to energy, pollution, and resource concentration"

Experimented with System Structures for Advanced Process Simulation
- with post-doc Babu Joseph

Used Plex (linked-list) data structures
- more flexible than dimensioned array structures

Information stored in beads of any length created from a dynamic pool of free storage – as needed during execution of programs

Beads point to the first addresses of other beads

Particularly effective for streams having different combinations of V, L_1, L_2, S phases

Created prototype PLEXSYS simulation program
- experimented with FORTRAN, PL1, APL, as the host language

Simulated coal gasification process with:
particle-size distributions
non-conventional components
different phase combinations

Larry and Warren visited simulation groups at 7 companies to gain feedback on PLEXSYS and its potential for next-generation simulators

Obtained seed money to build IEPES –
Integrated Energy Process Engineering System

Conducted a 2-day workshop on –
Modeling and Analysis of Industrial Energy Usage

Wrote proposal and obtained funding from DOE to develop the ASPEN simulator

Many PLEXSYS constructs eventually appeared in ASPEN

Many Related Activities – Larry and many others

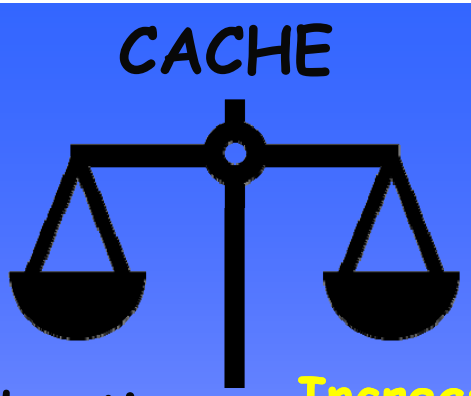
Richard R. Hughes proposed the Computing and Chemical Engineering journal

AIChE wasn't ready – Elsevier accepted.

1980 - Richard S. H. Mah and Warren Seider organized the FOCAPD Conference through the Engineering Foundation (created to facilitate conferences for the founding engineering societies)

New England College, difficult communications with facilitators, attendees, …

Early 1980s



Conferences Committee – R.S.H. Mah, Jeff Siirola

FOCAPD'1983 - Foundations of Computer-Aided Process Design

CPC III (1986) - Chemical Process Control

FOCAPO'1987 - Foundations of Computer-Aided Process Operations

Over 30 CACHE Conferences since 1983.

In parallel, Larry, his doctoral students, colleagues made research progress

Siri Jirapongphan – Simultaneous-modular convergence concept in process optimization

Chao-Chyun Chen – Chemical process simulation with electrolytes – extended Pitzer correlation

M. D. Barrera - Optimal Design and Operation of Batch Processes

A. Mulet - Pressure-vessel sizing and cost estimation
Amando Corripio

MIT 8-Day Summer Course – "Modeling, Simulation, and Optimization of Chemical Processes" ~20 years

To Larry –

Happy 80th Birthday!

It's my pleasure to acknowledge, with admiration and thanks, your many technical and managerial leading roles!