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DIAMOND SHAMROCK
Central Engineering

Diamond Shamrock Battleground Evaporator System

a

Perils of an Ancient Fortran IV Simulation

Don Harvey
Bob Fowler

March 13, 2025

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Area View from the Battleship Texas

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San Jacinto Battleground

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Battleground Quadruple Effect Caustic Evaporation System

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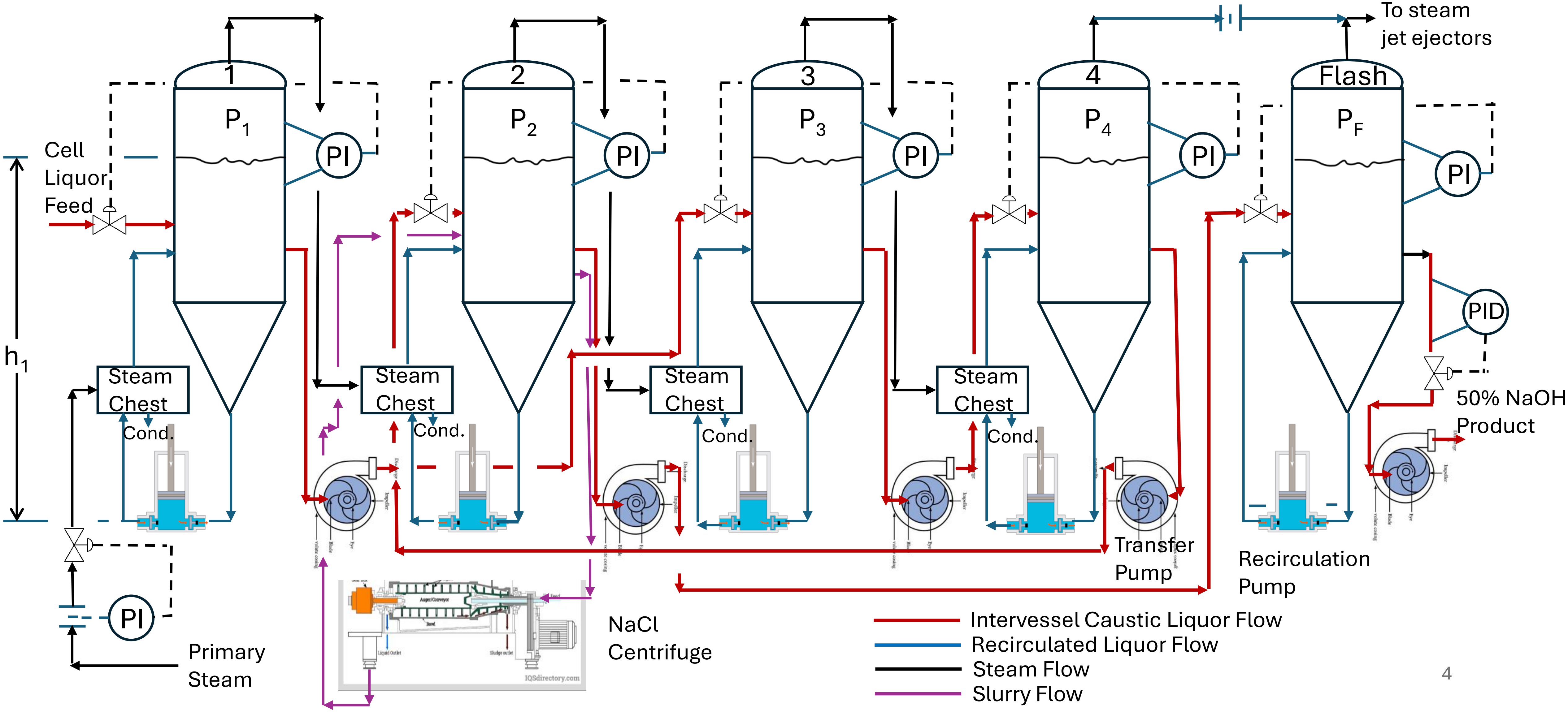

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The Scene of the Action—1200 t/d 50% NaOH Plant

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Diamond Shamrock's Battleground Plant in Houston, Texas.

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Management Concerns—Four Technical Objectives

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1. Determine Overall System Operability and Stability to Load & Set Point Changes & other Upsets
   - Confirm Corporate Investment—Failure was *not* an Option
2. Tune the Control System
3. Locate Bottlenecks
4. Find a Startup Method
   - No one had ever successfully started and operated such a complex plant
     - SS Operation was one Thing; dynamic Operation was totally unknown.
   - Cell Liquor would be used to Charge all Effects:
     - It was the resulting Liquor from electrolyzing NaCl Solutions
       a) Aqueous, approximately 10% NaCl, 10% NaOH
       b) Very different from SS Compositions in the Effects
       c) Desired Product 50% NaOH Aqueous Solution

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Who We Were in 1973

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- Dr. Don Harvey was an Assoc. Prof. of Chemical Engineering at CSU
  - His Specialty was Thermo but He taught a Course in Dynamic Simulation
  - He had met our Central Engineering Process Manager at a local Section AIChE Meeting and a Marriage was born!
  - Don was our Lead Engineer
- I started full Time at Diamond Shamrock on April Fool's Day, 1973. 😊
  - My graduate Work had been in Biochemical Engineering and Catalysis
  - The word *Simulation* (with IBM's CSMP) had appeared in my Resume but
  - I really had 0 Experience with *creating* simulation Software. However, ...
    - a) Simulation was in its infancy
    - b) No comprehensive canned Software available for Dynamic Modeling
    - c) No one Else available either, soooo

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We Got the Job!

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- Fantastic learning experience for me!
  - Essentially did a post-Doc under Don.
  - He is a Superb Engineer, Mentor and Friend!
  - And We were both young once! (🎼 🎶 Two Lovelier Fellows you never have seen!! 🎵)

- We developed a wonderful working Relationship and Friendship.
  - He had a little Experience with Simulation but a LOT with fundamental Chemical Engineering.
  - I knew a Little about the Operation of IBM Mainframes to go with my basic ChE education but very Little about creating Simulations.
  - We complemented each Other very well.

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The Schedule

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- The plant had been designed by Zaremba, Inc. of Buffalo, NY in the 60's
  - Quad Design thought to be very Energy efficient
- McKee Engineering (then a Stone's throw away from here over I77) was overseeing Construction in 1973 when we started
- Startup was scheduled for about Thanksgiving, 1974
- It was April, 1973, so we had about 1½ years to:
  - Write all Software from Scratch including all of the Simulator's Hardware and Physical Property Subroutines
  - Debug the Software
  - Get It to run dependably on an IBM Mainframe including
    - Finding reliable Convergence and Integration Methods
  - Confirm the Numbers on the P&ID ...
  - Meet all those Requirements set forth by Management

Simulator Creation

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The Givens

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1. **P&ID** with <u>*SS*</u> Conditions showing:
   i. Flow Rates
   ii. Compositions
   iii. Temperatures
2. **Physical Model** of the Plant at LaPorte
   i. Measured line lengths, number/type of fittings, etc. from this model
3. **Centrifugal Transfer Pump Curves**
   i. ΔP-Flow rate relationships with impeller diameters as parameters
4. **Control Valve Coefficients** (C_v) as Functions of Valve Stem Positions
5. **Roger Franks' Text**, *Modeling and Simulation in Chemical Engineering*, with fundamental software
6. **All Unit Ops** and other **Basic Expressions** and **Relationships**
7. **Physical Properties** (ρ, solubilities, BP's, P°, h's [single & multi ϕ, water])

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Software Tools

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1. Fortran II transitioned later to IV
2. Various curve fitting Techniques--Sometimes involved use of Paper Tape Input (!) to offline Computers
3. Minimal Experience with Numerical Methods but learned fast!
4. Wegstein and/or Half-Section for convergence
   - *Many* convergence Problems (steep Curves) from the start, so…
     - Transitioned to the slower Half Section Method if crazy Solution
     - Always Wegstein when Stability returned
     - Eventually developed Bounded Wegstein
5. Eventually used Newton-Raphson simultaneous multi-Variable Convergence with Numerical Estimation of the Jacobian for Effect Pressures

Software Tools (Cont'd)

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6. Integration by Euler or 4^{th} order Runge-Kutta
   - Reverted to RK4 exclusively as time went on
   - Systems were Invariably *Stiff* necessitating small Time Steps
     - Caused by subsystems with very different Time Constants
     - Time Step was increased with decreasing Integration Error Estimate
   - Ended up being very Reliable

Creating the Simulator

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Model Required Creation of Subroutines in Fortran IV for

- Physical Properties of all Process Materials (via Curve Fits)
  - Steam Tables
  - Solution Densities as a Function of Concentration
  - Solution Boiling Points
  - Solubilities (Ternary System Isotherms as Functions of Concentration)
  - Liquor Enthalpies as Functions of Concentrations and Temperature
- Pump and Valve Coefficient Curves
- PI and PID controllers (Franks offered introductory Examples)
- Flash Routines (given h and P, calculate T, ϕ's and Compositions)
- All kinds of other Utility Routines (e.g., Mix, Split, Pumps, etc.)
- Software to model System Flow Rates using "Electrical Analogy"

The Electrical Analogy (Flow-Head Relationships)

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Bernoulli Equation:

$\Delta P_p = (P_2 - P_1) + (\rho_g/g_c)(h_2 - h_1) + \Delta P_f$ (ΔP_p = Pump Pressure Rise)

Defn. of Friction Factor, f:

$\Delta P_{fl} = [v^2\rho/2g_c] \cdot [\Sigma L/D] \cdot f = R_l Q^2$ (Line, Manual Valve & Fitting Losses; Q=Vol. Flow Rate)

Control Valve Losses:

$\Delta P_{fv} = (Q/C_v)^2 \rho = R_v Q^2$

Total Line Friction Pressure Drop:

$\Delta P_f = \Delta P_{fl} + \Delta P_{fv} = (R_l + R_V)Q^2$ (Design: at least 35% of total ΔP_f through Control Valve at SS)

Rearranging the Bernoulli Equation results in:

$\Delta P_p - (P_2 - P_1) - (\rho_g/g_c)(h_2 - h_1) = Q^2(R_V + R_l)$ which is analogous to E = IR although Flow is squared. Kirchoff's Laws now apply.

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Programming Considerations

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1. The simulator needed to thoroughly model inherently non-linear flow-head Relationships (Electrical Analogy) & superimposed Heat Flows.
2. Differential Variables (those with long Time Constants) were determined.
   - All other Variables were solved for algebraically –
     - Saved Computer execution Time
     - Reasonable Approximation
3. Then Algebraic Equations are solved at Time 0 using Initial Conditions for Differential Variables
   - Differential Variables integrated to time t + Δt
   - Differential Variables updated followed by algebraic Solution of all other System Equations
   - Differential Variables re-integrated; repeat Process to Time t_{final}.

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System Calculations

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1. **Integrate Differential Variables at Time t+Δt**
   - Controller Signals → Control Valve Positions → R_V (R_l's fixed)
   - Vessel volumes → Vessel Levels (h_i)
   - Overall Compositions & Enthalpies → T_i
2. **Assume all Vessel Pressures**
3. **Solve all Heat and Material Balances Algebraically including**
   - Steam Generation in each Vessel
   - Flow Rates between Vessels
4. **Converge all Steam Pressures by comparing Steam Generated with Steam Consumed in next Vessel**
   - Done individually at first
   - Later simultaneously via Newton Raphson

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Running the Simulator

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All Runs were Batch using Punched Cards

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- Started a Batch run carrying Boxes of Cards from the 13th to the 12th Floor
  - Always hoping that we didn't drop Them!
  - Had to read 2 Boxes in every Time
    - Read in Main Program & all Subroutines including Physical Properties
      - ❑ Couldn't store *ANYTHING* on the Computer
- We submitted our Jobs into HASP's K, L or M Queues and waited
  - K, L & M Queues dedicated to Engineering
    - Increasingly large Slices of Physical Memory all the way up to ***250K!***
    - Always last Priority after Corporate Business Jobs
  - Virtual Memory not yet available
- Eventually our Runs required so much CPU Time that
  - We were forced to run Simulation Jobs at Night—One at a Time
  - Often negligible Results, so we waited until the next Night to run again.

Hardware Tools

- Our hardware tools consisted of
  - An IBM system/360 44 (no Software Storage or Virtual Capabilities)
    - Eventually a 370/158 Virtual Machine became available
  - IBM Cards
  - Card Punches
  - Card Readers
  - Line Printer
- No CRT's or anything else modern but those above were State of the Art
- No debugging or automatic Disk allocation capabilities available

Tools of the Trade

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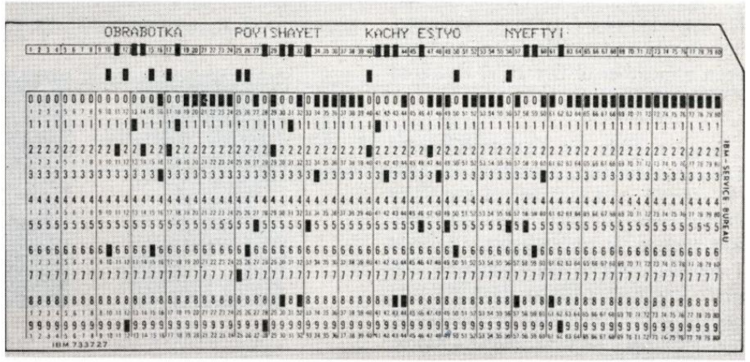

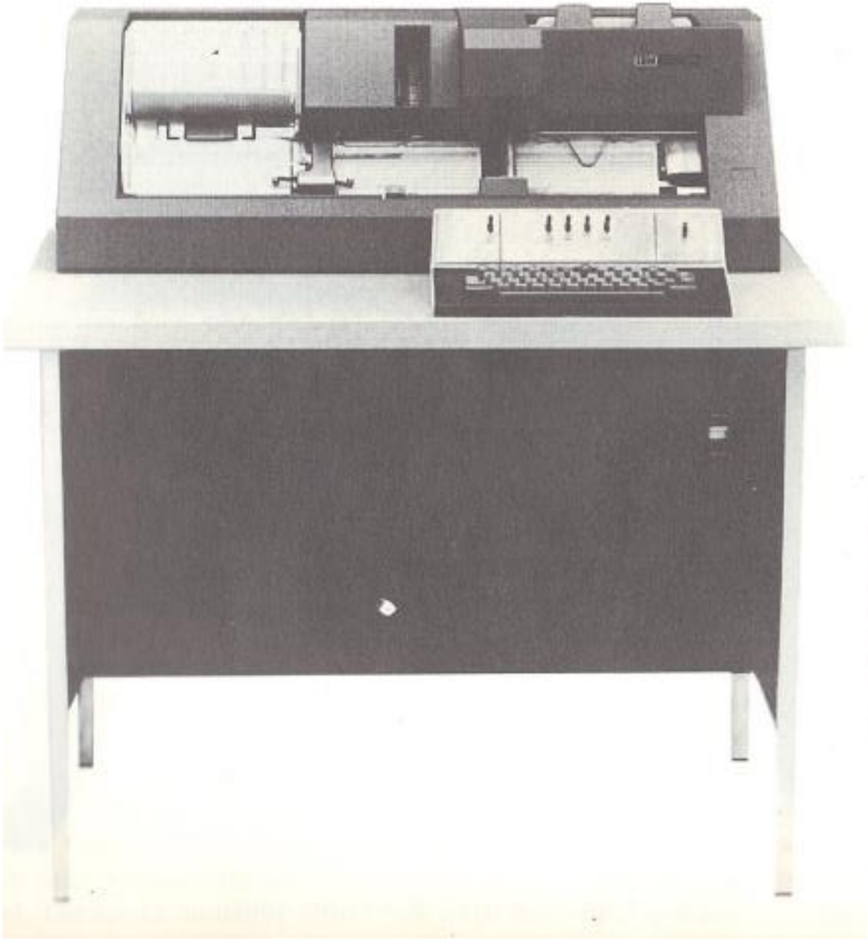

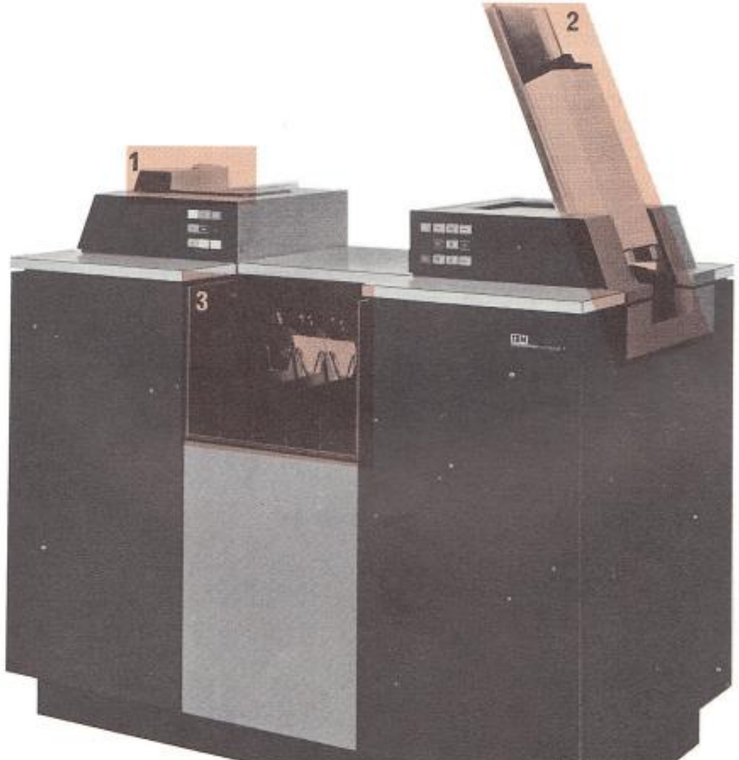

1. Punch input hopper
2. Read input hopper
3. Output stackers

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Fun with JCL

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1. Used to control Batch Runs and to create <u>inflexible</u> Disk Space "Data Sets"
2. Commands used with IBM *Job Control Language* (JCL):
   a. JOB, EXEC, DD, ENDJOB.
   b. Had to *learn* and extract JCL Routines from a Multi Volume Manual
3. Consequences of Use
   a. Frequent Overruns of Results <u>filled Data Sets and stopped Execution</u>
      i. Needed to constantly delete and create new, larger Data Sets since ***All*** Commands had to be given to the Computer manually.
         - The Operating System wasn't designed to perform ***any*** of these Tasks on its own.
      ii. Typical Data Set command: something like *Disp=(End, Catlg, Delete)*
4. A CSU Grad Student, (now) Dr. Paul Husted, eventually aided us with JCL
5. IEFBR14—Drove us up a Wall!!

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The JCL Conundrum

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Overlay Structures

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- Eventually the Program wouldn’t fit into any Allocated Physical Computer Memory space
  - When this happened, Everything literally stopped.
- With the 360/44 had to learn to manually create “Overlay” Structures
  - *Groups* of Subroutines (specified by us) which the Computer swapped into and out of available Physical Memory as the Program ran
- Problems:
  - Had to basically regroup the Software—also drove us up a Wall!
    - Took substantial amounts of Time to set up
  - Values of Variables weren't kept as Routines were swapped in and out
    - Necessitated putting almost all Variables into Common Blocks
- Not an issue of course with Modern, Virtual Memory Computers

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Debugging

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- ***The*** Major, very Time-consuming Issue
- Division by 0 was a constant Problem
- Problem Indicator: Hex Program Location Indicator (what's that?)
- Our Most Effective debugging Method
  - This Technique Indicated the *Proximity* of the Problem.

With such a large program, Don and I were sometimes so confused by the Nature of the Bug that, on a nice Day, we were known to go down to the little Shop on the ground Floor, buy a Bag of Doritos, go outside and walk around the Block sharing them to clear our heads!

THE most Insidious Bug

😟

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```
Call Subroutine A ( x, 2, y, z...)
-----------------------------------------
    Subroutine A ( x, i, y, z...)
        x = y + 2.
        i = i + 1
        z = 3. + y
    Return
    End
-----------------------------------------
j = 2
Print "j = ", j
-----------------------------------------
j = ?
```

- **REALLY** drove us to eat Doritos!!
- It took us **DAYS** to find this one.
- It's an Access Violation—not allowed by modern Computers

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Results

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Output

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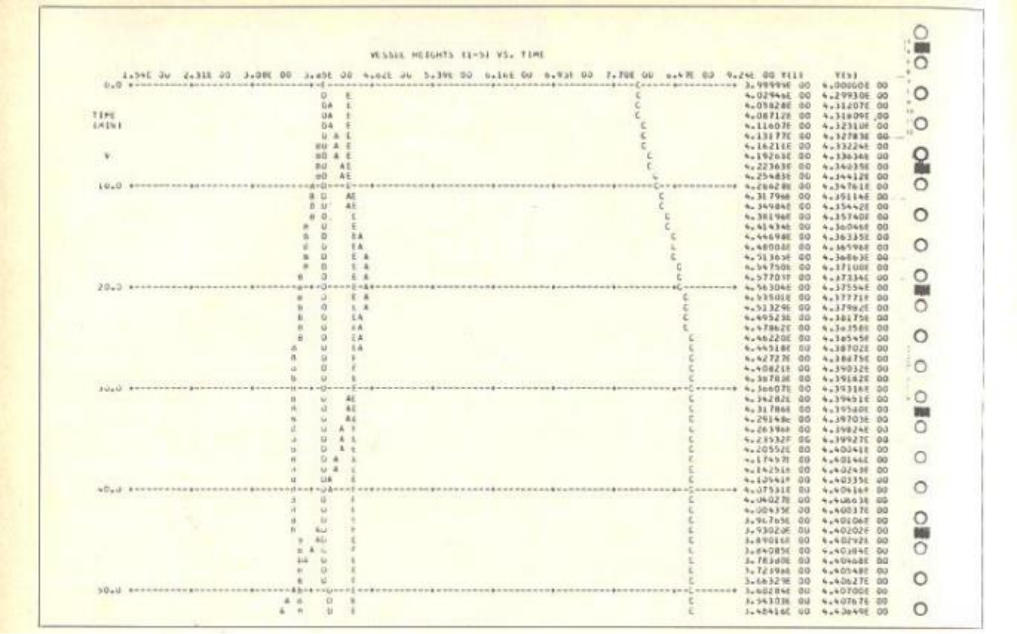
- Our sole Output was 132 character-wide printed Sheets
- Output Information from 5 Vessels included
  - Temperatures
  - Pressures
  - Flow rates
  - Compositions
  - Slurry Concentrations
  - Liquid Levels
  - Control Valve Positions



- The Conference Room Happening!
- It was literally a Technical Luxury

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Program Progress

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- Basic Software written relatively early on
  - Kept adding to it as Time went on
- Except for minor Issues with our Software and Convergence and Integration Issues, the basic Simulator was complete by late 1973 or early 1974.
- First interested in
  - Confirming the basic Design
  - Tuning the Control System
  - Confirming System Stability
- At this point, Problems which occurred with the Simulator’s Performance were relatively mild.
- And then there were ....

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Our Customers

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- Term includes HQ Divisional Engineers and all Plant Engineers
- *Very* skeptical of how these two Pointy Heads with their fancy Software and ***no in-plant Experience*** could assist Them in their *real World*.
    - VERY *real Problem*!!
    - During this initial Phase of Software Development, the Plant was still under Construction.
    - Often times we suggested Design Modifications
        - Especially with the Impeller Sizes of the Centrifugal Transfer Pumps
        - Our Model showed that they were invariably too small to accommodate even modest transient Conditions
    - Issues: (1) Every Surface exposed to the hot Caustic/Salt Solutions was made of expensive Nickel
      (2) Larger Impellers more costly to operate.

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Startup Simulation

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- Starting such complex Plant had never been attempted by Anyone Anywhere
- The First Step was to meet with the Customers, their Drawings and Grease Pencils.
  - They told us how They *would have* started the Plant—Step by Step.
  - We loaded their Conditions into our Simulator.
- Their Startup conditions:
  - Had to use Cell Liquor everywhere because higher Concentration Liquors had never been produced there
    - Apparently it was impractical to truck some of similar Concentrations (and Elevated Temperatures) in from Elsewhere
    - But using Cell Liquor everywhere was *far removed* from SS conditions
  - Customers insisted that Controller Settings not be Changed from SS
  - Primary Steam only—Steam for other effects unavailable initially.

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Startup Simulation (II)

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We entered the Customers' Suggested Startup Procedure into the Model

- Immediately encountered ***MAJOR*** Issues:
  - Salt built up in the 1st Effect where there was no way to remove it.
  - Sluggish Control System was totally incapable of handling Startup Conditions in automatic.
    - So the plant would have to be started manually with the Control System eased back to automatic as the Effects approached steady state. Fairly easy to model with the Simulator.
  - Issues with the Levels in several Effects—especially the Third Effect, but we were able to *manually* control them all.
- Any of these would have stopped Operations in its Tracks.
- All these Issues were unanticipated but became obvious as the Customers thought about Them.

Startup Simulation (III)

- Customers finally agreed that... WOW!! ...
  - These *were indeed* **major** Issues that they hadn't anticipated which would have cost them major Downtime to analyze, clean up and fix.
- Faith in our Simulator was in its Infancy but their Skepticism started to wane!
- Example of a Fix:
  - Totally unanticipated Water Line to the First Effect proved necessary to keep the Salt in Solution as the First Effect lined out.
    - *Imagine*: the Effects were designed to *remove* Water, and now we were deliberately *adding* Water to one of Them!
- We developed Guidelines for when Manual Control was to be initiated and then discontinued
- Even included a home-made PD controller.

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Startup Simulation (IV)

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- The Customers had closely followed the Results of our Progress in creating a Workable Startup Process, solving Problem by Problem (usually one per night).
- Over time they realized our Model made sense and had uncovered a Myriad of unanticipated Process Issues.
  - They totally bought into our Results
  - No more Skepticism!!
  - Working together, we worked out Fixes for ***every*** Problem ***before*** Construction was complete and the actual Startup initiated
- In the End we created a complete, step-by-step Startup Hard-copy Manual which was issued to all interested parties.
- It became the “Startup Bible”.

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The Actual Startup

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- After a Year and half of Development, Testing and Working with the Customers, we were all ready to go.
- During Startup Don and I stayed in Cleveland, close to the Computer just in case ☺ (there was certainly no WWW in those Days!).
- We were on Long-distance[1] for the entire Afternoon and Evening of the first Train's Startup.
- All of the corporate big wigs, including the CEO, were present in the Control Room for the Startup holding their collective Breaths. I think.

[1]The expensive, old-fashioned type of Long-distance

Startup Problems

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The actual Sequence of Events closely matched those predicted by our "Startup Bible" as Startup commenced, buuut…

- The Level in the First Effect went off script and kept dropping.
- At one Point They reported to us that the Level in the Third Effect was rising to dangerous Levels.
- Beyond that there was a Physical Problem with Gaskets in one of the Control Valves that delayed the Startup.
- But that was it.
- In the end, the Plant basically started in one Shift.
- Maybe Management breathed a Sign of Relief—but They didn't tell Us.
- But I did get a couple of Tickets to a Browns Game. 😁

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The Finale

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- One day I had a chat with the Liaison Engineer for the responsible Operating Division, Diamond's ElectroChem Division:
- I casually mentioned to Him that we thought we had saved the Corporation a few million Bucks in Startup Costs (including negligible Downtime).
- The Guy looked at me and said, "Don't ever tell *Them* that!"
- I started to say Something, but He added "*They* think You saved Them $60M" (1974)! —about $400M today.
- The alleged DuPont Story.
- It was a wonderful Start to this Engineer's Career!
- Thanks for Everything Don!!
- And Thanks To Our Customers For Their Support!!!

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And Thank You for Listening.

How about some Easy Questions?