[redacted]

# PROJECT ADVISORY COMMITTEE - SYSTEMS ANALYSIS

and

# MAPPS USER'S GROUP

## SLIDE MATERIAL

March 26-27 1986

MAINFRAME VERSION

9 users

Full implementation on:

IBM Series 3xxx & 4xxx machines

Burroughs B6910

VAX 11/780

MASSCOMP MCS510

µMAPPS

IBM PC, XT, AT

COMPAQ

## DIFFERENCE BETWEEN MICRO AND MAINFRAME VERSIONS

Help menus

Problem size - floppy disk versions

FORTRAN 77 vs. FORTRAN 66

Execution speed

Accuracy

## SPEED COMPARISONS

Generic Pulp Mill

| | |
|---|---|
| B6910 | 45 sec |
| VAX 11/780 | |
| MASSCOMP | 45 sec |
| PC/XT | 260 sec |
| PC/AT | 130 |

FUTURE:

Same code on μ & mainframe

FORTRAN 77

Revised file handling

Revised help menus

## NEW MODELS

STAFF DEVELOPED:

Supported

Documentation & code distributed

STUDENT DEVELOPED:

Not supported

Available by request

Copy charge for M.S. thesis

Thesis contains model descriptions, code, and worksheets

## SUPPORTED MODULES

RATIO

- Computes ratio of module or stream parameters
- Documentation distributed
- Included with original source

STMHTR

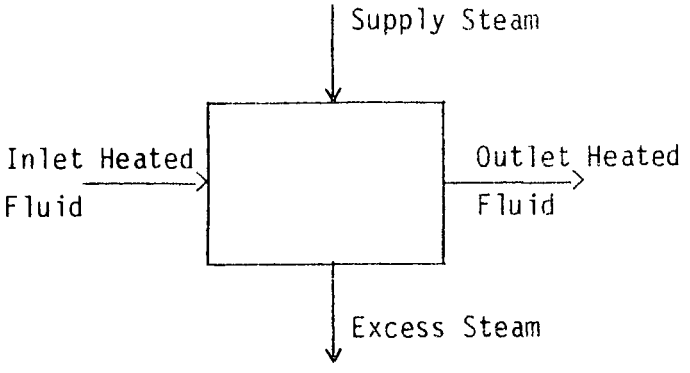
- Direct steam heater
- Code and documentation to be distributed

RPRTØ1

- Simple report generator
- Code and documentation to be distributed

STMHTR

· Models a direct steam heater.




· Description:

A calculated amount of steam is added to a heated fluid stream to raise the temperature of the stream.

Given:

(a) Desired exit fluid temperature

or

(b) Desired temperature rise

Calculated:

(a) Amount of required steam

RPRTØ1

A) Prints out summary information on a group of streams being used in the simulation.

B) Either ALL streams or a user specified group of streams may be requested.

Statistics reported:

1) mass flow rate (lb/hr or kg/hr)

2) total flow rate (gal/min or L/s)

3) consistency, %

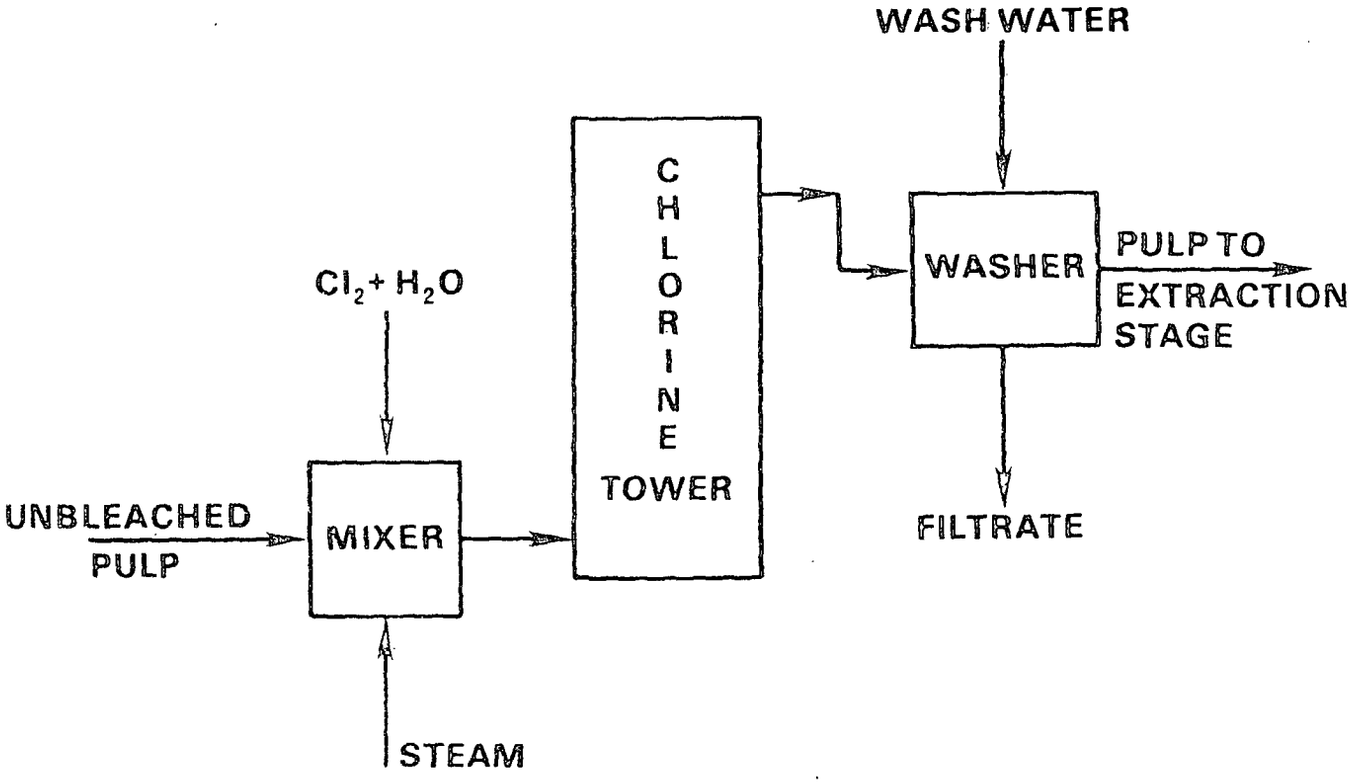
4) dissolved solids, %

MAPPS

Bleaching Models

- Chlorination
- Extraction
- Chlorine dioxide bleaching

## CHLORINATION



CHLORINATION KINETICS

$$-\frac{d(XLF)}{dt} = k_1(XLF)(CL2) \quad \text{FAST}$$

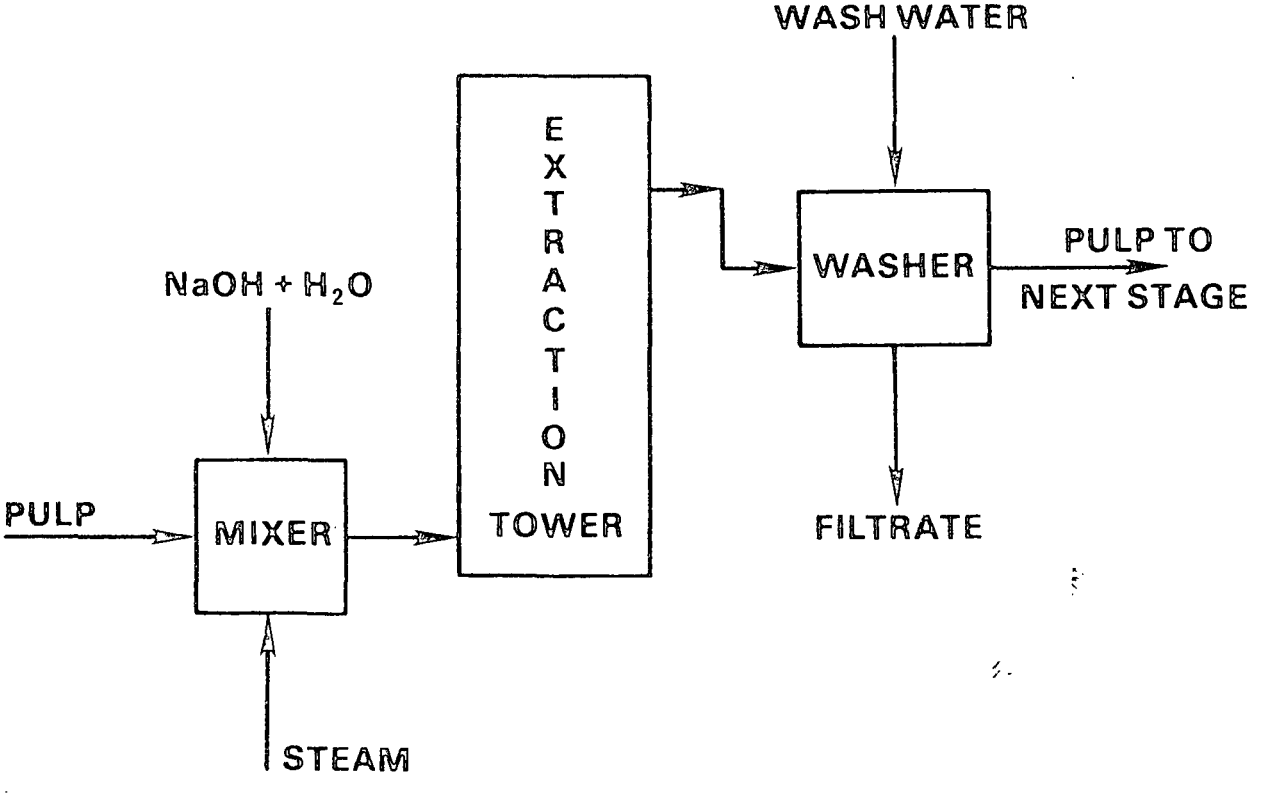
$$-\frac{d(XLS)}{dt} = k_2(XLS)(CL2) \quad \text{SLOW}$$

$$XL + a\,Cl_2 \rightleftharpoons b\,XLC + c\,HCl$$

Lignin Chlorolignin

Ackert, et al., Tappi 58:141 (Oct., 1975).

# EXTRACTION



## $ClO_2$ BLEACHING: D1 and D2 STAGES

$$-\frac{dC_k}{dt} = K[ClO_2]^{0.5}\,[H^+]^{-0.3}\,[C_k - C_{k\infty}]^3$$

$$\frac{d[ClO_2]}{dC_k} = \frac{K_3}{C_k^n}, \quad \begin{matrix} n = 1, \text{ D1 stage} \\ = 2.3, \text{ D2 stage} \end{matrix}$$

Teder and Tormund (1) CPPA Trans. Tech. Section 3:41(1977), (2) AIChE Symp. Series, Vol. 76, No. 200, p. 133(1980).

## CHLORINATION

User supplied data:

- Input stream No. 1 (washed pulp)
- Input stream No. 2 ($Cl_2$ + $H_2O$)
- Input stream No. 3 (steam/$H_2O$)
- Chlorine tower volume

Optional information:

- Rate constants
- Stoichiometric data
- Mass balance factors

## CHLORINATION

Output

- Stream No. 4 (chlorinated pulp)
- Retention time (hours)
- Total conversion of lignin
- Residual chlorine
- Temperature of reactor

STUDENT MODULES:

Sam Busch - April, 1984
A Computer Model of a Multiple Effect Evaporator

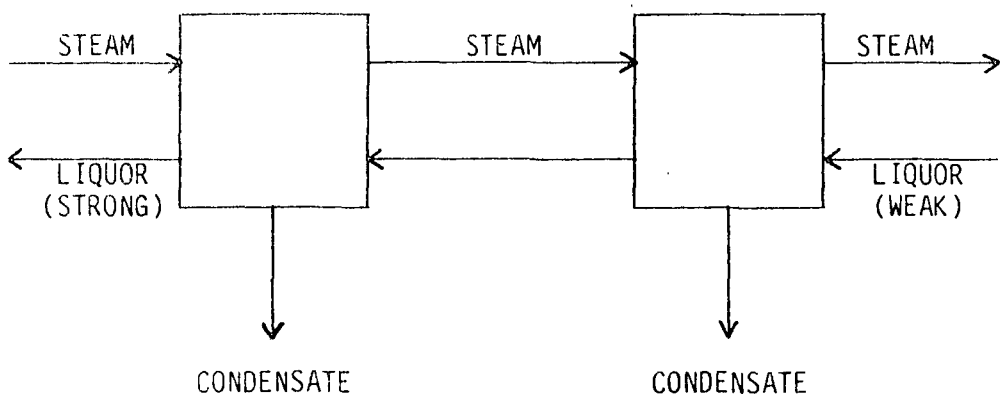
Greg Kulas - March 5, 1985
The Development of an Oxygen Stage Bleaching Model for MAPPS

STUDENT MODULES (Contd.):

Arlene Heaster - Dec. 11, 1984
A MAPPS Model of the Chemical Conversion Cycle in an Alkaline Sulfite-Anthraquinone Pulp Mill

Scott Dibbs - Feb. 22, 1985
Modeling and Simulation of the Alkaline Sulfite-Anthraquinone Pulping System

EVAPORATOR MODEL




| CONVENTIONAL | BUSCH |
|---|---|
| SPECIFY: | SPECIFY: |
| WEAK LIQUOR | STRONG LIQUOR |
| FEED STEAM | FEED STEAM |
| EXCHANGER DESIGN | EXCHANGER DESIGN |
| ITERATE: | ITERATE: |
| EACH MODULE UNTIL CONVERGED | FEED STEAM FLOW TO DESIRED WEAK LIQUOR CONCENTRATION |

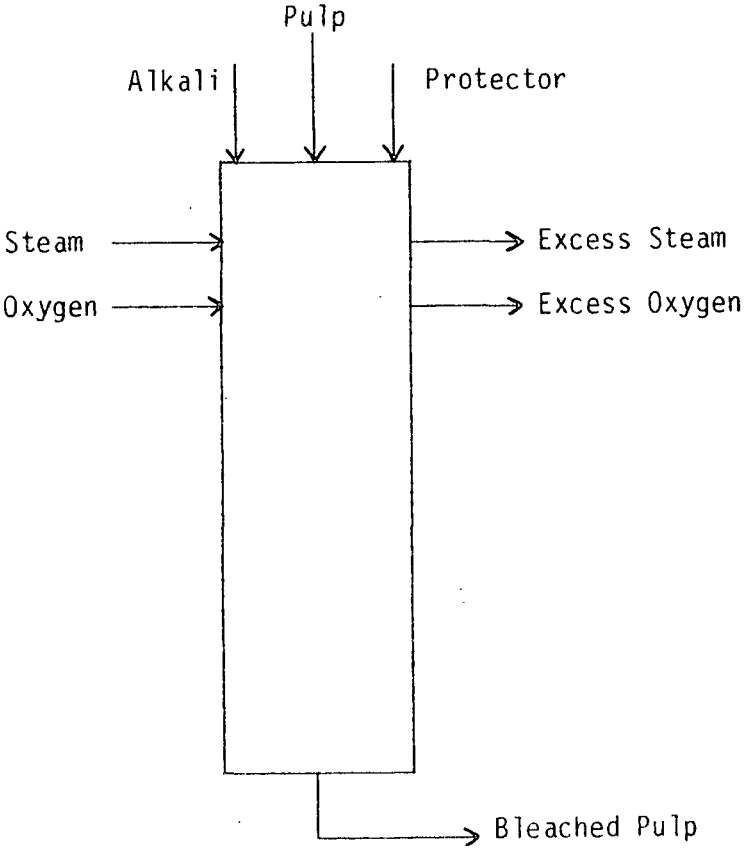
ADVANTAGES:

No iterative calculations except for control on steam flow.

DISADVANTAGES:

Must specify desired weak liquor concentration.

OXYGEN BLEACHING



## OXYGEN BLEACHING

Down flow tower

Assumptions:

Plug flow

Isothermal

Protected carbohydrate

Convective transport only

Reactions as outlined by Olm & Teder, Tappi 62(12): 48-46(Dec. 1979)

Constant oxygen pressure

## OXYGEN BLEACHING

Basic Kinetics:

Lignin = Slow + Fast = $L_s + L_f$

Slow rate = $k_1 (OH^-)^{0.3} P_{O_2}^{0.2} \cdot L_s$

Fast rate = $k_2 (OH^-)^{0.1} P_{O_2}^{0.1} \cdot L_f$

## OXYGEN BLEACHING

Carbohydrate Degradation (as viscosity loss):

Slow rate = $k_3 (OH^-)^{0.6} P_{O_2}^{0.1}$

Fast rate = $k_4 (OH^-)^{0.2} P_{O_2}^{0.8}$

Fast ——> Slow when 85% of fast lignin removed

## ALKALINE SULFITE-ANTHRAQUINONE SYSTEM

Pulping:

Modified kraft digester

Modified white liquor controller

Modified makeup controller

Modified recovery furnace

Recovery:

Tampella-Rauma System

ASAQ MODULE

Pulping:

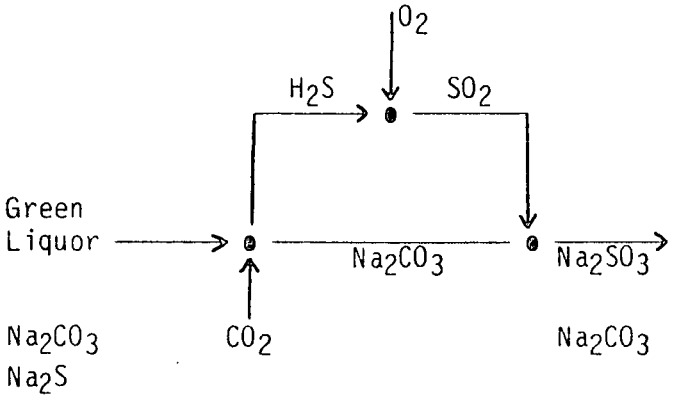
DIGRØ4

WLIQØ2

MKUPØ2

ASAQ

Recovery Cycle:



ASAQ MODULES

Recovery:

ABSORB

$SO_2$ Absorption

$CO_2$ Stripping

Reactions:

$$SO_3^{=} + SO_2 + H_2O \longrightarrow 2HSO3^{-}$$

$$2HCO_3^{-} \longrightarrow CO_3^{=} + CO_2\uparrow + H_2O$$

$$2HSO_3^{-} + CO_3^{=} \longrightarrow 2SO_3^{=} + CO_2\uparrow$$

$$HSO_3^{-} + HCO_3^{-} \longrightarrow SO_3^{=} + CO_2\uparrow H_2O$$

ASAQ MODULES

Recovery:

CARB

Carbonates green liquor

Reactions:

$$CO_3^{=} + CO_2 + H_2O \longrightarrow 2HCO_3^{-}$$

ASAQ MODULES

Recovery:

H2STRP

Forms and strips $H_2S$

Reactions:

$$HCO_3^- + HS^- \longrightarrow CO_3^= + H_2S\uparrow$$

ASAQ MODULES

Recovery:

PRCARB

Green liquor precarbonation

Reactions:

$$2\ S^= + CO_2 + H_2O \longrightarrow 2\ HS^- + CO_3^=$$

$$CO_3^= + CO_2 + H_2O \longrightarrow 2HCO_3^-$$

ASAQ MODULES

Recovery:

SO3TON

Sulfitation of green liquor

Reactions:

$$2HSO_3^- + CO_3^= \longrightarrow 2\ SO_3^= + CO_2\uparrow$$

$$HSO_3^- + HCO_3^- \longrightarrow SO_3^= + CO_2\uparrow$$

MAPPS FORTRAN 77

CONVERSION OBJECTIVES

1. Convert code to FORTRAN 77 for portability and long-term compiler support.

2. Produce a mainframe version of MAPPS that can be easily transported to a micro.

3. Take advantage of the file handling capabilities of FORTRAN 77.

4. Add customer recommendations.

IBM has discontinued support

of level G and H compilers.

After conversion to FORTRAN 77, MAPPS would still not run on the PC using the MS-FORTRAN compiler.

Reasons:

1. The stack, format statements, and arrays declared "NOTLARGE" are stored in one 64K segment.

2. Arrays that are declared "LARGE" and are initialized via DATA statements in subroutines "disappear."

S O L U T I O N S

1. ALL of the "prompt mode" routines were eliminated, except those needed for the MAKE command.

   The user can obtain help by calling up disk-based menus.

   Example: HELP
   HELP ADD

MAPPS MASTER MENU

HELP IS AVAILABLE FOR THE FOLLOWING COMMANDS:

SUPERVISORY COMMANDS
 CANCEL  ECHO  END  STATUS

FILE COMMANDS
 COMPARE  COUNT  GET  SAVE  NEW  ERASE

EDIT COMMANDS
 ADD  CHANGE  DELETE  MAKE  REMOVE

WRITE COMMANDS
 DISPLAY  PRINT

EXECUTE COMMANDS
 RUN

+ TO GET MORE INFORMATION, ENTER HELP FOLLOWED BY THE SECTION NAME OR COMMAND NAME

STRUCTURE OF THE ADD COMMAND IS:

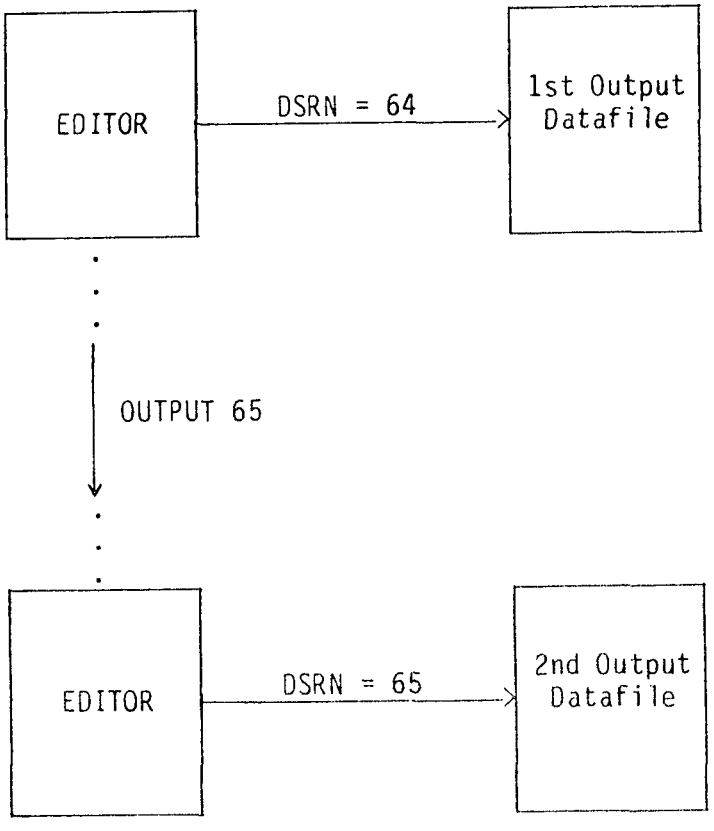
| COMMAND | | ACTION |
|---|---|---|
| ADD | MODULE N | ADDS MODULE "N" TO THE DATA FILE. MODULE DATA ARE REQUESTED. |
| ADD | STREAM N | ADDS STREAM "N" TO THE DATA FILE. STREAM DATA ARE REQUESTED. |
| ADD | DEFINITION N | DEVELOPS A NEW COMPONENT DEFINITION FOR STREAM TYPE "N". A NEW DEFINITION IS REQUESTED. |
| ADD | TITLE N | ADDS THE NTH TITLE LINE TO THE DATA FILE. N MUST BE 1, 2, OR 3. A NEW TITLE STRING IS REQUESTED. |
| ADD | ORDER | INSERTS MODULES IN THE CALCULATION ORDER. STARTING POINT AND MODULES ARE REQUESTED. |

2. The prompts for the MAKE command are retained, but they are also disk based.

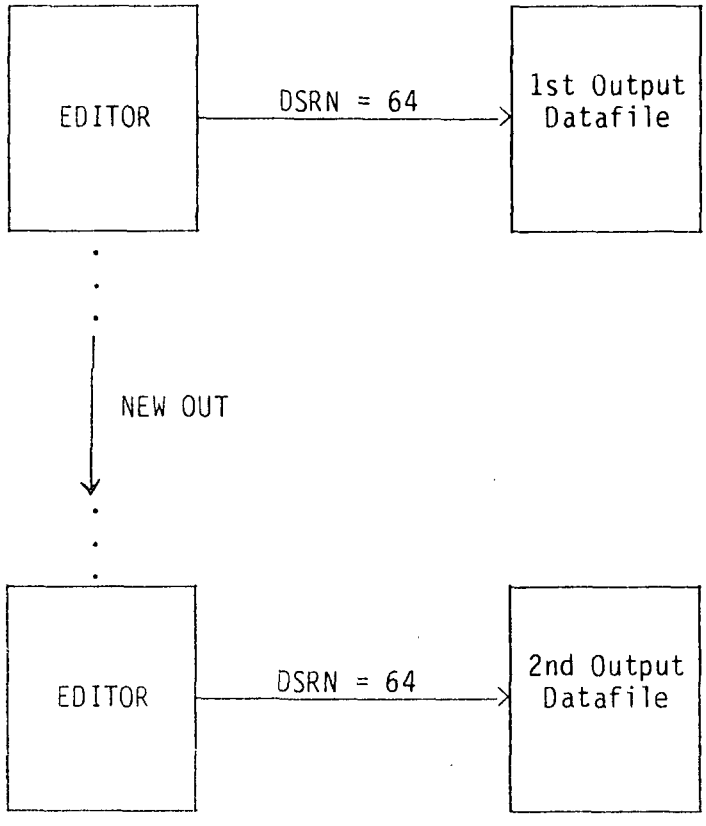
3. Most initializations of arrays via DATA statements were replaced by assignment statements. The arrays in the remaining DATA statements must be declared "NOTLARGE" in the micro version.

The FORTRAN 77 version of MAPPS offers improved run time file handling.

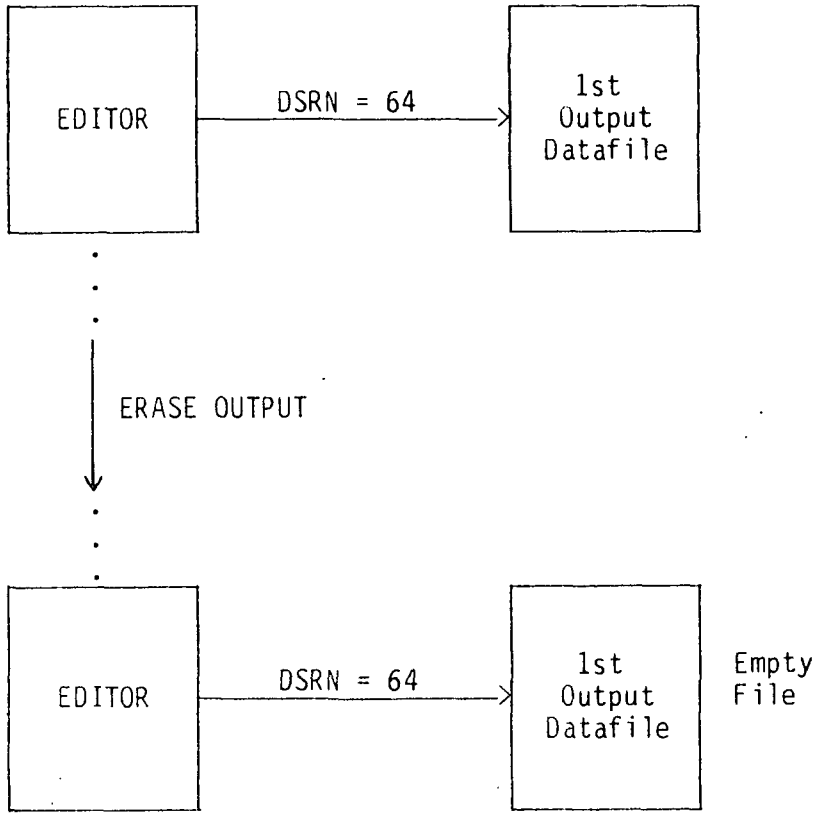
Run time file handling in MAPPS Release 1.0



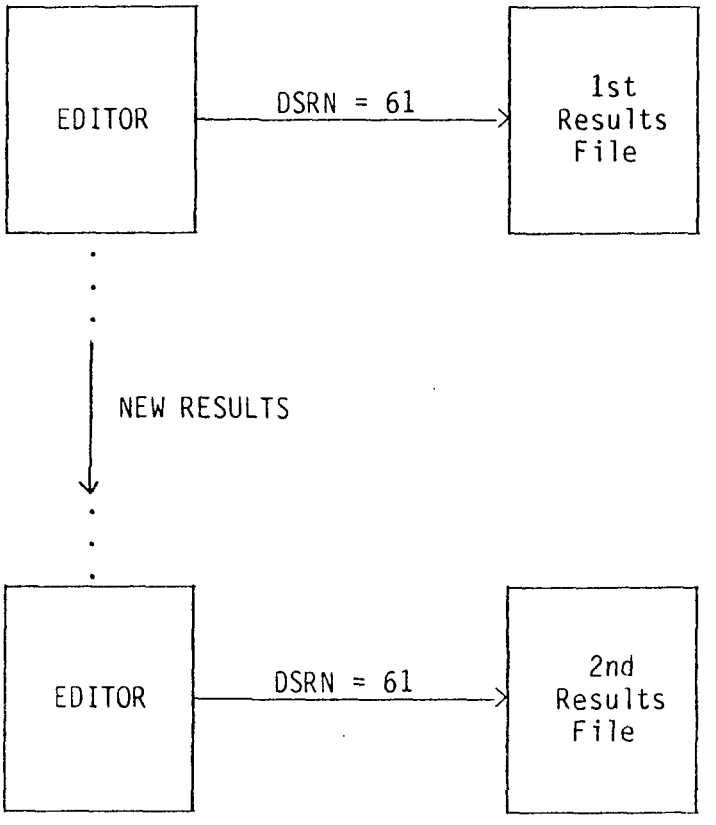
Run time file handling in MAPPS Release 1.1
(FORTRAN 77)



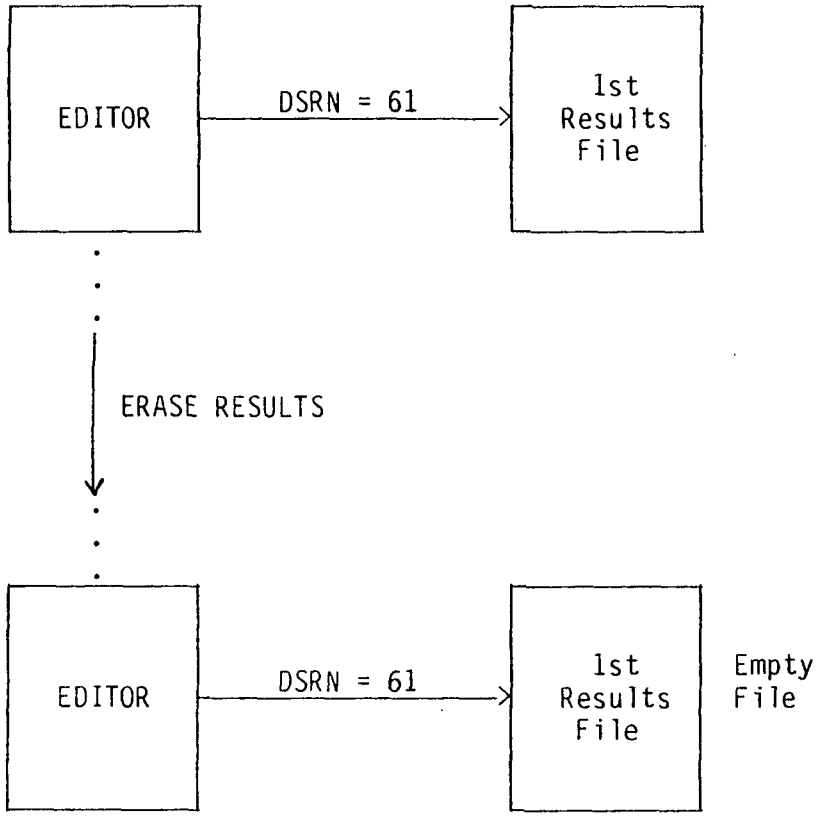
Run time file handling in MAPPS Release 1.1
(FORTRAN 77)



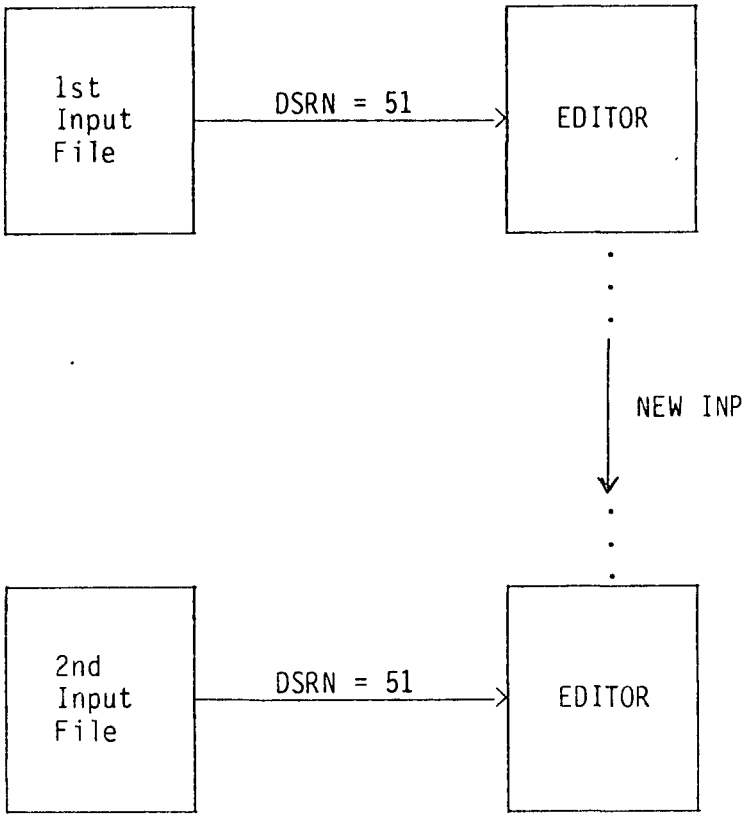
Run time file handling in MAPPS Release 1.1
(FORTRAN 77)



Run time file handling in MAPPS Release 1.1
(FORTRAN 77)



Run time file handling in MAPPS Release 1.1
(FORTRAN 77)



Allow multiple parameter or parameter ranges on a command line.

Example: DIS MOD 14 1, 3, 11-17

Displays parameters 1, 3, and 11 through 17 for module 14.

RUN ORD 1-5

Runs the modules in the calculation order positions 1 through 5.

Improve the information content of error warning messages.

Old message:

```
* WARNING ** MODULE  11 : STREAM
44 HAS A NEGATIVE FLOW RATE
```

New message:

```
* WARNING ** DESUP  11 : STREAM
44 FLOW =      -61.654
```

MAPPS PERFORMANCE COMPARISONS

CPU TIME REQUIRED TO EXECUTE
THE GENERIC PULP MILL

| | |
|---|---|
| MAINFRAME | |
| FORTRAN 66 | 39 SEC |
| FORTRAN 77 | 76 SEC |
| MICRO | |
| IBM AT | 120 SEC |
| IBM XT | 250 SEC |