FINAL REPORT
FOR PROJECT PERIOD

SYSTEMS ANALYSIS OF CHEMICALS AND
ENERGY RECOVERY IN SULFATE PULPING

PROJECT 2893
SEPTEMBER 15, 1969 - SEPTEMBER 14, 1971

Prepared by
PROJECT STAFF

Graduate Students - Purdue University
Lewis S. Adler
Peter M. Chase
Frode L. Galtung
Edgar F. Jacobi
Michael V. Kotik
Laxmi K. Rastogi
Clifford C. Smith

Staff Members - Institute of Paper Chemistry
Dr. Thomas M. Grace
Dr. Robert A. Holm
FOREWORD

The undersigned wish to use this opportunity to express their gratitude and thanks to Dr. Donald A. Brewster of the Westvaco Corporation (now with Measurex, Inc.) who had the original idea for carrying out this project and who was instrumental in completing the arrangements between the Institute of Paper Chemistry and Purdue University which made it possible.

We wish also to thank the sixteen sponsoring companies of the project and particularly their representatives who attended our several reporting meetings and guided our efforts throughout the period of the research. All of us are also especially grateful to those companies who received our students during the 1969 and 1970 summer periods to obtain data for their studies. Plant personnel at all these plants were very helpful to the students in their work.

The contributions of Dr. Rolf Isermann of the University of Stuttgart and Professor Antti Niemi of the University of Helsinki in modelling the multiple effect evaporators is acknowledged with our special thanks.

Robert A. Holm, Director
Division of Industrial and Environmental Systems
Institute of Paper Chemistry

Theodore J. Williams, Director
Purdue Laboratory for Applied Industrial Control
Purdue University
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CONCLUSIONS

This Report presents our estimate of the best set of mathematical models for each of the units of the chemical and energy recovery section of a paper mill except for the brown stock washers. This latter element is covered in the separate report of Dr. John F. Perry (1). Presented also is an outline of the control system judged to take best advantage of the information available from the use of these models and of the proposed instrumentation system also stated herein. The proposed control system was developed with the digital computer in mind and would be difficult to implement with any other type of control element for the overall control system.

Once implemented the proposed control system should be able to present the following advantages to the mill installing such a system:

1. Provide a continually updated steady-state economic optimization of the operation of the total chemical and energy recovery unit based upon that operational production criterion which exists at the moment: maximum production, maximum profit, or minimum cost.

2. Permit continual operation of the Kamyr digester at either the highest possible yields or at the maximum pulp production possible with the available raw wood stock.

3. Reduce drastically the variation in solids composition of the black liquor throughput when limited evaporation
steam is available. Reduce to a small fraction the amount of weak black liquor storage necessary to assure smooth operation of the evaporator system.

4. Assure the highest possible smelt reduction under any imposed operational condition. Make possible the highest attainable energy recovery through steam production. Reduce the necessary manpower commitment for recovery furnace operation. Improve furnace operational safety by maintaining char bed level and providing fast alarm in case of possible black-out conditions.

5. Preserve those operating conditions in the causticizers and settlers which will assure the highest possible conversion of alkali and the fastest settling of causticizer reaction solid products.

6. Determine and maintain the best operating conditions for the lime kiln as a function of overall required caustic availability and production rate.

In addition to the continual total economic optimization of the operation of the overall pulp, chemicals, and energy recovery units the following gains should be possible through use of the proposed control system.

1. Reduction of salt cake addition to a minimum by allowing a maximum reduction ratio i in the furnace and minimizing sodium and sulfur losses in washing operations and furnace flue gases.
2. Reduction of fuel costs in the lime kiln through reduction of quick lime production with higher efficiency and better settling in the causticizing operation.

3. Minimization of steam costs through reduction of wash water flows and of process water requirements in the digester.

All of these capabilities have been demonstrated by computer simulation during the progress of the research reported herein. However, since each student studied a different type of plant unit and in a different plant environment during his period of summer study it is difficult to assign total dollars saving values which should be possible as a result of the eventual implementation of the recommendations for the control system design which is developed in this report. Such a determination would, of course, be readily possible with a particular consistent set of plant characteristics, operating parameters, and economic performance data for a specific pulp mill.
REFERENCES CITED

SECTION I
INTRODUCTION

ORIGIN AND OPERATION OF THE PROJECT

This project on Systems Analysis of Chemicals and Energy Recovery in Sulfate Pulping was submitted as Research Proposal 1476 of the Institute of Paper Chemistry, Appleton, Wisconsin, for a joint study between the Division of Industrial and Environmental Systems of the Institute and the Purdue Laboratory for Applied Industrial Control of Purdue University, Lafayette, Indiana. It was funded by a group of sixteen companies as follows:

American Can Company
Neenah, Wisconsin 54956
Mr. B. G. Klowak, Representative

Consolidated Papers, Incorporated
Wisconsin Rapids, Wisconsin 54494
Dr. I. Bruce Sanborn, Representative

Container Corporation of America
Brewton, Alabama 36426
Mr. George H. Whiteside, Representative

Crown Zellerbach Corporation
Camas, Washington 98607
Dr. Mark A. Hannah, Representative

Great Northern Paper Company
Millinocket, Maine 04462
Mr. Paul D. Hubbe, Representative

Green Bay Packaging, Incorporated
Green Bay, Wisconsin 54305
Mr. William R. Relson, Representative
The major work of the project was carried out by a group of engineering graduate students of Purdue University under the
supervision of the staff members from Purdue University and from
the Institute of Paper Chemistry. Each of these students used
the research involved here as part of his requirements for the
degree of Doctor of Philosophy in Engineering at Purdue. The
exception to this was the separate work of Dr. John F. Perry of the
Institute of Paper Chemistry (now Kimberley-Clark Corporation,
Neenah, Wisconsin) on the dynamics of brown stock washers. His
work has previously been published by the Institute of Paper
Chemistry as Report One, Project 2893, "Preliminary Mathematical
of this earlier work, the area of brown stock washer dynamics and
control is not specifically treated in this Report.

During the project period several of the students spent a
period of one summer collecting in-plant operating data on their
particular phase of the study. For the following students the
summer of 1970 was spent at the mills listed:

<table>
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<th>Company</th>
</tr>
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<tbody>
<tr>
<td>Louis S. Adler</td>
<td>Consolidated Papers, Incorporated Wisconsin Rapids, Wisconsin</td>
</tr>
<tr>
<td>Peter M. Chase</td>
<td>American Can Company Halsey, Oregon</td>
</tr>
<tr>
<td>Frode L. Galtung</td>
<td>Owens-Illinois, Incorporation Valdosta, Georgia</td>
</tr>
<tr>
<td>Michael V. Kotik</td>
<td>Crown Zellerbach Corporation Clatskanie, Oregon</td>
</tr>
</tbody>
</table>

Previous to this Clifford C. Smith had spent the summer of 1969
at Westvaco Corporation, North Charleston, South Carolina. These
summer study-work periods were invaluable to the students for
obtaining on insight into the operation of industry in general and
of the chemical recovery process, in particular, as well as providing
the means for obtaining plant data necessary for their later work.
OBJECTIVES OF THE PROJECT

The main objective of the proposed project was established to critically evaluate how to get the most profit from the application of process control to the kraft recovery system. Additional benefits would result from the clearer understanding of the interdependence of the units in the recovery system. A better understanding of the sources of chemical loss would also contribute to future efforts to limit these emissions and decrease the pollution load on air and water treatment facilities.

It was noted that the kraft pulp industry currently spends more than $30,000,000 annually on chemicals make-up in its mills. Operating methods or control schemes which would result in even a small improvement in efficiency would more than repay the investment and effort required in this study.

The study was proposed as a cooperative research program between The Institute of Paper Chemistry and the Purdue Laboratory for Applied Industrial Control. Each of these organizations has a unique capability which was to be brought to bear on the problem of decreasing chemicals loss and increasing energy recovery from the complex, interdependent system of washing, evaporation, burning, dissolving, causticizing, clarifying, and calcining. The project would proceed through the development of accurate mathematical models of each of the processing units in the system. The detail included in each unit was to depend on available knowledge and the requirements of the work. After the complete system was modelled, a sensitivity analysis was to be performed to determine which of the material and energy flows had the largest effect on the overall
economics of recovery.

In this way those parts of the process which could contribute most to an increase in the efficiency of operation would be identified and these parts of the process examined in greater detail. In this way the effect of individual unit and complete integrated system control on the recovery process could be investigated and useful estimates could be made of benefits and costs of better control.

Extensions of this work to more accurate descriptions of the economically-important process units, the evaluation of more powerful control schemes, and the integrated model of a bleached-kraft pulp mill would then be possible.

Integrated process analysis, or systems engineering, has previously been applied to several parts of the pulp and paper-making process (1, 2). Initial applications have been in the areas of blending and stock preparation, paper machine operation, pulping, and bleaching (3). The field of chemical recovery has been relatively neglected up until now. This is possibly due to the complexity of the interactions and to lack of knowledge of the behavior of the individual units in the recovery system. Although our knowledge of the individual unit behavior is increasing, little work had yet been done on the complete system. That such work was needed is evident in the observation of interactions of the units in the system which cannot be adequately treated by considering only the behavior of the individual process units. The chemical recovery system in a kraft mill is illustrated by Figure 1, which is a simplified schematic drawing of the interrelationships of the major process components.
Nomenclature

1. Digester 8. Direct-Contact Evaporator
3. Knotters and Washers 10. Smelt Dissolving Tank
4. Foam Tank 11. G.L. Storage
5. Weak B.L. Storage 12. G.L. Clarifier
7. Strong B.L. Storage 14. W.L. Clarifier

15. W.L. Storage 16. Cooking Liquor
17. Precipitator 18. Turbines
19. Dregs Washer 20. Mud Washer
21. Lime Kiln

FIGURE 1
SULFATE PULPING AND RECOVERY SYSTEM
There are many benefits to be derived from the smooth, controllable operation of the recovery system. In addition to obtaining the profitable recovery of chemicals and energy, the operation of the recovery system affects the quality and uniformity of the pulp which is produced and the operating efficiency of subsequent manufacturing processes. Additional important advantages of proper control are the coupled benefits of obtaining maximum chemical recovery and concomitantly decreasing the pollution load on air or water-treatment facilities. Proper control can also increase the average throughput of the recovery system, permitting the same system to handle a higher pulp load or a higher dilution load for a given production rate. The overall controllability and safety of the recovery system are additional very important aspects which may be closely tied to the complete control problem.

To determine where to most profitably apply process control in chemical recovery, one must know the static and dynamic behavior of the equipment and processes to a useful degree of accuracy, and be able to test the effect of proposed operating procedures or control schemes.

Although information has been available on the operation and control of several of the individual process units in the chemicals area, such as evaporators or kilns, there has been no general study of the operation of the entire integrated system prior to this project. Since the chemical recovery cycle involves large amounts of recycled material and energy, there are opportunities for optimization of the entire system which are completely missed by an individual unit approach. It was expected that many opportunities for application
of these advanced control techniques would present themselves as soon as the mathematical models of the various plant units were formulated.

There are a number of variations in piping arrangements and operating conditions from one kraft mill to another. A process engineer must be able to adjust the system to correspond to each individual mill arrangement. In this project, this was to be made possible by developing an accurate description of each individual unit in the recovery system on a modular basis. These component modules would then form a set of mutually compatible "blocks" which would describe, to the required degree of accuracy, the steady-state and dynamic behavior of the pulping reactors, washers, evaporators, recovery furnace, kiln and other units. The piping and flow arrangements external to the individual units could then be arranged in any particular application to correspond to individual mill requirements. When properly connected, these individual unit descriptions form a mathematical model of the pulping and recovery system which can be tested by computer simulation techniques to determine its sensitivity to various operating variables(4).
OUTLINE OF WORK CARRIED OUT

The following is an outline of the major areas of work included in this project. It will be seen that it approximates very closely that included in Proposal 1476.

A. Steady-State Modelling of Entire Recovery System
   1. Agreement on overall system flow chart of process areas to be considered and interconnections to be treated. Identification of major process variables for steady state model.
   2. Development of overall steady state model for a typical process arrangement. Formulation as a linear programming model and exercise of this model to determine initial sensitivity of system to economic and operational factors.

B. Dynamic Mathematical Modelling of Individual Components
   3. Identification of the major external and intercomponent dynamic variables which would allow the compatible use of the module in the integrated system.
   4. Modelling of the dynamic behavior of each individual process area according to the following procedure:
      (a) Critical literature survey of articles on unit response and treatment of related units from other industries.
      (b) Contacts with equipment manufacturers for descriptive and dynamic data.
      (c) Consultation with an Advisory Committee of industry representatives regarding features to
be described by the mathematical model.

(d) Selection of specific typical process units to be modelled.

(e) Definition and mathematical description of dynamic behavior of the unit.

(f) Computer programming and simulation (analog, digital, and hybrid computers) of the unit dynamic behavior from the mathematical model.

(g) Comparison of simulated with actual plant behavior. Modification of mathematical model as necessary to duplicate actual plant test data.

C. Economic Behavior of the Integrated Chemical Recovery System

5. Combination of area models into an overall mathematical model of the chemical recovery plant cycle.

6. Consultation with the Advisory Committee, to define operational and economic upsets, which may affect the dynamic operation of the chemical recovery plant cycle.

7. Testing of the economic response of the chemical recovery plant cycle by simulation of the mathematical model for realistic economic and operational upsets.

D. Formulation and Testing of Control Schemes

8. Formulation of best overall control scheme for the chemical recovery plant cycle. Development of probable economic return to be realized from the control system.
9. Review of instrumentation required to implement such a control system.
ADDITIONAL REPORTING OF RESEARCH RESULTS

As mentioned earlier each of the students presently involved in the research work of this study is working toward the Doctor of Philosophy degree in Engineering at Purdue University. As such each has or will prepare a detailed report of his research accomplishments as his thesis for this degree. These reports will be published by the Purdue Laboratory for Applied Industrial Control and will be distributed to the contributors to this Project as further reports of the work.

The work of Frode L. Galtung on A Mathematical Model and Digital Computer Based Advanced Control System for a Kraft Mill Recovery Unit, has already been distributed as Report No. 43 of the Laboratory. The work of Lewis S. Adler, Economic Optimization of a Kraft Recovery Cycle, is nearing completion and should be available in early 1972 as Report No. 48 of the Laboratory. That of the others; Clifford C. Smith, Peter M. Chase, Laxmi Rastogi and Edgar F. Jacobi, should follow within the next year or so depending upon their total educational progress toward their degree.

In each case the present report presents the methods used, the conclusions reached, and the major results to be presented in each thesis. Because of lack of space in this single report, more detail on that particular aspect of the project will be presented in each individual thesis report.
REFERENCES CITED


SECTION II
PROPOSED CONTROL SYSTEM

GENERAL

As stated earlier this project has three major goals which are:

1. Model the overall system in a steady-state manner suitable for economic optimizing or supervisory control.

2. Model each individual unit dynamically to develop the necessary information to propose an advanced dynamic control system capable of significantly improving present control practices in this industry.

3. Develop proposals for when and where possible benefits are to be obtained from the required control systems for each unit and the overall process.

Our resulting proposal for the control system will be developed in this Section. The required mathematical models appear in the following Sections (III - VIII).

Figure 1 of Section III, page 119, summarizes the major external variables of recovery systems.

As will be seen in the detailed discussions to follow, the proposed control systems are in most cases too complex for implementation to be attempted with conventional analog control hardware. Thus a digital computer-based, control system is proposed herein. Because of the nature of the control functions involved, a two level system is proposed (Figure 1) consisting of a dual-minicomputer type unit working under a large supervisory control...
FIGURE 1

PROPOSED DIGITAL CONTROL SYSTEM
CHEMICALS AND ENERGY RECOVERY SECTION OF A PAPER MILL
The dual-minicomputer type unit will handle the proposed dynamic control schemes for each unit of the Recovery Section. A dual computer is proposed to help assure the necessary system reliability to attain a dependable continuation of the benefits inherent in this system and decrease the likelihood of interruptions to the process. Such installations are now quite common in the chemical, petroleum, metals, and power industries, and are finding increased acceptance in the pulp and paper industry.

The supervisory level computer will handle the economic optimization proposed with the steady state model of Section III. Such a work load would require only a fraction of the computing capability of such a machine. Thus it could be used to carry out similar management control functions for the wood yard, stock preparation, paper machine, and product inventory sections of the complete paper or board mill.

While both types of functions could be carried out in a dual computer system of sufficient size, cost factors will dictate that the proposed system would probably give the highest cost effectiveness rating for these systems. However, as of this writing, we have not attempted to develop a specific machine configuration and price for such a system.

In contrast to the physical layout of the digital computer system as depicted in Figure 1, Figure 2 presents a functional concept of the control system to be presented herein. The supervisory level computer confines itself, as mentioned earlier, to the steady state economic optimization described in the next part.
of this Section. All phases of the special advanced control algorithms developed for dynamic control and the computation of valve motion via direct digital control (DDC) algorithms will take place in the subordinate dynamic control computers (the twin minicomputer system of Figure 1). Note that no advanced control algorithms are proposed for the black liquor oxidizer or causticizing units. This is due to a lack of data and consequent detailed study of the oxidizer unit. In the case of the causticizer unit it is shown in Section VII that proper operation of the Kiln depends upon operating conditions in the former unit. Thus advanced control of these two units in considered together in the proposals.
DEVELOPMENT AND EXECUTION OF THE ECONOMIC (STEADY-STATE) OPTIMIZATION OF THE OVERALL KRAFT RECOVERY CYCLE

A steady-state or algebraic economic optimization of the total kraft recovery cycle process is proposed here because of the overall complexity involved and the consequent load on the computing resources available from the usual process control type computer. Of first importance for such a task is the development of the performance function to be minimized (if expressed as costs) or maximized (if expressed as profits). Depending upon its complexity and that of the model used in conjunction with it (Section III) a solution scheme is developed. Our proposals for both of these for this project are presented below.

The reader is directed to the Symbols Used listing of Section III for the definition of symbols used here. Several examples of the formulation, use, and results obtained from the optimization performance function, plant model, and solution scheme proposed here will be found in the additional Report of Adler and Goodson (1).
FORMULATION OF THE PERFORMANCE FUNCTION FOR THE STEADY-STATE OPTIMIZATION

As previously stated, a specific objective of this Project has been to develop a means to determine the optimum set points which will minimize the operational cost of running the kraft mill on a day-to-day basis. Therefore, the physical condition of each piece of equipment is important and is accounted for in the model. Since the cost of the machinery, equipment and other fixed costs does not affect the production efficiency, this parameter is not included in the performance index. The main components of the performance function to be derived here are the cost of gaseous and particulate emissions in terms of an emissions penalty, the cost of makeup chemicals in terms of their purchasing price, the production and use of energy in the form of steam, the cost of wood chips and the profit in pulp production. The cost function is based on the production of one ton of air dry pulp.

It is extremely important to emphasize that the cost coefficients presented here are not intended to reflect the prices associated to a particular component by any specific paper company. However, the cost figures do represent "typical" kraft mill revenue and expenditure rates and are the results of averaging data from several sources. It is the responsibility of each company which chooses to use the results of this work to assign their own specific costs to the various coefficients.

The units for the cost function are $/tadp. In some cases variables have to be converted from one set of units to another; the conversion factors are included in the formulation.
DIGESTER MODULE

The costs for the digester module include the price of wood chips, the cost of steam and wash water, the revenue from pulp production and a penalty function used to define practical operating ranges. Thus, the cost performance function for the digester module can be expressed as the following linear relationship.

\[ F_I = C_{wc} U(15) + 60 C_{st} (Y(4) + Y(5) + 1154.2Y(18))/ADTP + 60 C_{H_2O} W(bt)/ADTP - C_{pulp} + PENLT1 \]  

(1)

where the first term is the cost of delivery of wood chips to the digester, the second term is the cost of steam energy consumption, the third term is the cost of using process water from the filtrate plant and the next to last term is the revenue gained from the production of pulp. The constant 1154.2 is the energy of the saturated steam to the steaming vessel at 18 psia. The factor ADTP stands for tons of pulp per hour and is computed as

\[ ADTP = 60 Y(1)/2000 \]  

(2)

Note that expenditures are expressed as positive terms in the performance index; thus, the optimization will attempt to minimize this cost function. Table I on the next page lists the cost coefficients and their assigned values.

The last term is a three part penalty function for violating certain constraints which must be met in the operation of the digester module. These functions operate to effectively constrain operating variables by applying high cost penalties for operation
TABLE I
COST COEFFICIENTS

<table>
<thead>
<tr>
<th>Cost Coefficient</th>
<th>Value</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>$C_{\text{CaO}}$</td>
<td>0.01</td>
<td>$/\text{lb}$</td>
</tr>
<tr>
<td>$C_{\text{CH}_4}$</td>
<td>0.015</td>
<td>$/\text{lb}$</td>
</tr>
<tr>
<td>$C_{\text{H}_2\text{O}}$</td>
<td>100.</td>
<td>$/10^6\text{gal}$</td>
</tr>
<tr>
<td>$C_{\text{H}_2\text{S}}$</td>
<td>1,10,100.</td>
<td>$/\text{lb}$</td>
</tr>
<tr>
<td>$C_{\text{NaOH}}$</td>
<td>0.03</td>
<td>$/\text{lb}$</td>
</tr>
<tr>
<td>$C_{\text{Na}_2\text{SO}_4}$</td>
<td>1,10,100.</td>
<td>$/\text{lb}$</td>
</tr>
<tr>
<td>$C_{\text{pulp}}$</td>
<td>160.</td>
<td>$/\text{tdnp}$</td>
</tr>
<tr>
<td>$C_{\text{RSH}}$</td>
<td>1,10,100.</td>
<td>$/\text{lb}$</td>
</tr>
<tr>
<td>$C_{\text{RSR}}$</td>
<td>1,10,100.</td>
<td>$/\text{lb}$</td>
</tr>
<tr>
<td>$C_{\text{RSSR}}$</td>
<td>1,10,100.</td>
<td>$/\text{lb}$</td>
</tr>
<tr>
<td>$C_{\text{SC}}$</td>
<td>0.014</td>
<td>$/\text{lb}$</td>
</tr>
<tr>
<td>$C_{\text{SO}_2}$</td>
<td>1,10,100.</td>
<td>$/\text{lb}$</td>
</tr>
<tr>
<td>$C_{\text{ST}}$</td>
<td>1.5</td>
<td>$/10^6\text{Btu}$</td>
</tr>
<tr>
<td>$C_{\text{WC}}$</td>
<td>100.</td>
<td>$/\text{ton}$</td>
</tr>
</tbody>
</table>
outside of a given range. First, the consistency of the pulp leaving the drum of the brown stock washer must be between 0.11 and 0.13 lb. pulp/lb. total flow prior to repulping. Thus,

\[
\text{if } 0.11 \leq \frac{X_{\text{bw}}}{F} \leq 0.13 \quad (3)
\]

\[
F_c = 0
\]

\[
\text{if } \frac{X_{\text{bw}}}{F} < 0.11 \text{ or } \frac{X_{\text{bw}}}{F} > 0.13 \quad (4)
\]

\[
F_c = 10^4
\]

where \(X_{\text{bw}}\) represents the lb. pulp/lb. total flow leaving the washer drum.

Also, the consistency of the blow flow is limited to maximum value of 0.2. Thus,

\[
\text{if } \frac{X_{\text{d}}}{F} \leq 0.2 \quad (5)
\]

\[
F_{cd} = 0
\]

\[
\text{if } \frac{X_{\text{d}}}{F} > 0.2 \quad (6)
\]

\[
F_{cd} = 10^4
\]

Finally, the K number for the pulp is restricted to the range of 75-80. Thus,

\[
\text{if } 75 \leq K \leq 80 \quad (7)
\]

\[
F_k = 0
\]
if \( K \leq 75 \) or \( K \geq 80 \) \hspace{1cm} (8)

\[ F_k = 10^4 \]

where the \( K \) number is computed as

\[ K = \frac{100Y(2)}{0.153} \]

Thus, the penalty portion of the performance function is

\[ \text{PENLT1} = F_c + F_{cd} + F_k \] \hspace{1cm} (9)

**EVAPORATOR MODULE**

The performance function for the evaporator module consists of the costs for steam usage, gas and vapor emissions, and the production of condensate which can be used as process water.

\[ F_2 = C_{st} \cdot U(2) \cdot H^{(ev)}_{st} / ADTP + C_{H_2S} \cdot H_2S^{(ev)} + C_{SO_2} \cdot SO_2^{(ev)} \]

\[ + C_{RSH} \cdot W_{RSH} + C_{RSR} \cdot W_{RSR} + C_{RSSR} \cdot W_{RSSR} \]

\[ - C_{H_2O}^{(ev)} \cdot ADTP \] \hspace{1cm} (10)

The first term is the cost of steam used and the last term is the credit given for useful condensate. Because the model is charged for process water used at the filters and washers, it is also consistent to credit the production of condensate since it is assumed to be relatively free of contamination by liquor. The remaining terms are the costs of chemical emissions as pollutants.

**FURNACE MODULE**

The cost index for the furnace module includes the addition
of salt cake at the cascade evaporator, the steam production and usage, pollutant emissions and again a process penalty function.

\[ F_3 = \left[ C_{H_2S} X_F(7) + R_{H_2S} \right] + C_{SO_2} X_F(8) \]

\[ + C_{Na_2SO_4} \left[ PFC \cdot X_F(11) + PFS \cdot X_F(12) \right] (1 - K_{pc}) \]

\[ + C_{sc} U(3) + C_{st} \left[ w_{st}(h, h) - w_{st}(f, f) \right] \] + PENLT3 (11)

The first three terms represent the cost of emitting the gaseous pollutants, hydrogen sulfide and sulfur dioxide, and the particulates, sodium carbonate and sodium sulfate. The fourth term is the cost of salt cake. The next-to-last terms are the charges for using and producing steam energy.

At the Consolidated mill, which was most closely investigated, the steam produced by the furnace is combined with steam produced by two coal-fed boiler systems and piped to a three stage turbine for electrical power generation. Since the ratio of recovery furnace steam to total steam supply to the turbogenerator varies, it is not possible to include the generation of electrical power in the cost optimization. However, at mills where only furnace steam is used for the turbine system, this additional revenue and cost should be included in the cost function.

The last term in Equation 11 is a penalty function which is a constraint on the optimization. A requirement for safe recovery furnace operation is that the percent solids in the black liquor leaving the cascade evaporator be in the range 60-66%. Thus,
if \[0.60 \leq x^{(ce)}_{\text{bils}} \leq 0.66\] (12)  
PENLT3 = 0

if \[x^{(ce)}_{\text{bils}} < 0.60 \text{ or } x^{(ce)}_{\text{bils}} > 0.66\] (13)  
PENLT3 = 10^4

GREEN LIQUOR CLARIFICATION MODULE

The cost function for the green liquor clarification module accounts for the use of plant water at the smelt tank and dregs filter, the cost for dumping dregs, and a penalty function. With the information from Table II the chemical losses at the dregs filter can be computed.

sodium: \[w^{(df)}_{\text{Na}} x^{(df)}_{\text{Na}} = (1 - \eta_{\text{glc}})(1 - k_f) [0.434 \times G(1) + 0.59 \times G(2) + 0.324 \times G(3)] + 0.00235 w_{\text{dregs}}\] (14)

where the constant coefficients in the first term represent the ratio of the atomic weights of sodium in the compound to the weight of the compound represented by the state variable.

sulfur: \[w^{(df)}_{\text{S}} x^{(df)}_{\text{S}} = (1 - \eta_{\text{glc}})(1 - k_f) [0.41 \times G(2) + 0.225 \times G(3)] + 0.024 w_{\text{dregs}}\] (15)

lime: \[w^{(df)}_{\text{CaO}} x^{(df)}_{\text{CaO}} = 0.332 w_{\text{dregs}}\] (16)
TABLE II
ASSUMED CHEMICAL DISTRIBUTION OF
GREEN LIQUOR DREGS

<table>
<thead>
<tr>
<th>Chemical</th>
<th>Percent by weight in dregs</th>
</tr>
</thead>
<tbody>
<tr>
<td>CaO</td>
<td>33.2</td>
</tr>
<tr>
<td>Na</td>
<td>2.35</td>
</tr>
<tr>
<td>S</td>
<td>2.4</td>
</tr>
</tbody>
</table>
Some mills convey the dregs to the lime kiln where they are burned. At the Consolidated mill the dregs are trucked to a predetermined location for disposal. It will be assumed that the small cost of deposition of the dregs is approximately equal to the penalty for sodium sulfate emissions. Thus, the performance index is

\[ F^4 = C_{Na_2SO_4} \cdot W_d (df) (X_{Na}^d + X_{S}^d + X_{CaO}^d) \]

\[ + C_{H_2O} \cdot [U(8) + U(9)] + PENLT^4 \]  \hspace{1cm} (17)

The last term in Equation 17 is a penalty function which will force the optimization to maintain the density of the green liquor leaving the smelt tank in the range 20-22°Be which corresponds to a density of 70.35-74.35 lb/ft\(^3\). Therefore,

\[ \text{if} \quad 70.35 \leq \rho_{gl} \leq 74.35 \]

\[ \text{then} \quad PENLT^4 = 0 \]  \hspace{1cm} (18)

\[ \text{if} \quad \rho_{gl} < 70.35 \text{ or } \rho_{gl} > 74.35 \]

\[ \text{then} \quad PENLT^4 = 10^4 \]  \hspace{1cm} (19)

CAUSTICIZING MODULE

The cost performance function for the causticizing module consists of the costs for plant water usage, new lime addition at the slaker-classifier, fuel supply to the kiln and the penalty
for hydrogen sulfide emission by the kiln.

\[ F5 = C_{CaO}W_{nl} + C_{H_2O}U(4) + C_{CH_4}U(10) \]

\[ + 0.2 C_{H_2S} - C_{CaO}W^{(ex)} \]  

where the constant 0.2 represents a typical value for hydrogen sulfide emissions/tadp (2, 3). The last term accounts for the possibility of the kiln producing more lime than is required.

MAKEUP MODULE

The cost function for the makeup module consists of the amount of sodium hydroxide, sodium sulfide and plant water which is required to adjust the white liquor to the conditions specified by the optimization. Also included is a possible revenue for producing excess white liquor:

\[ F6 = C_{H_2O} [W_{W}(mu) - EXWL(4)] - C_{NaOH} [W_{NaOH}(mu) + W_{Na_2S}(mu) - EXWL(2)] \]

\[ \quad - EXWL(5) \]  

where the first term is the trade-off between water usage and water in excess white liquor, the second term represents the profit in producing sodium carbonate and sodium sulfate in the excess white liquor and the last term is the difference between adding sodium hydroxide and sodium sulfide versus producing extra amounts of these two chemicals in the excess white liquor. It is assumed that the costs of sodium carbonate and sodium sulfate are the same;
also sodium sulfide and sodium hydroxide are assumed to have the same market value. Finally, from related equations in Section III.

\[ w_{\text{w}}^{(\text{mu})} = w_{\text{w}}^{(\text{mul})} + w_{\text{w}}^{(\text{mu2})} \]  \hspace{1cm} (22)

\[ w_{\text{NaOH}}^{(\text{mu})} = w_{\text{NaOH}}^{(\text{mul})} + w_{\text{NaOH}}^{(\text{mu2})} \]  \hspace{1cm} (23)

\[ w_{\text{Na}_2\text{S}}^{(\text{mu})} = w_{\text{Na}_2\text{S}}^{(\text{mul})} + w_{\text{Na}_2\text{S}}^{(\text{mu2})} \]  \hspace{1cm} (24)
OPTIMIZATION TECHNIQUE EMPLOYED

The technique employed for the optimization is a Hooke-Jeeves pattern search. The advantages of using this method are:

(1) it is well-suited to non-linear problems; and (2) gradient computations are not required, only a single function evaluation at selected points is performed. The programming used for the optimization package and following discussion were taken from Software Report No. 70-10SW, of Electronic Associates, Inc., Princeton, N. J. (4).

The first step in the pattern search method begins with a local exploration at an arbitrary base point \( b_1 = (U(1), U(2), \ldots, U(24)) \). A schematic diagram of the procedure is shown in Figure 3. The variable \( U(i) \) is perturbed in the positive direction by an amount \( \Delta U(i) \), the remaining control variables remaining unchanged, and the performance function \( F \) is evaluated. If \( F(U(i) + \Delta U(i)) \) is less than \( F(U(i)) \), then a new base point is established at \( U(1), U(2), \ldots, U(i) + \Delta U(i), \ldots, U(24) \). \( \Delta U(i) \) is an initial step size specified by the user as a percent of the range over which \( U(i) \) may vary.

If \( F(U(i) + \Delta U(i)) \) is not less than \( F(U(i)) \), then the value of the performance function at \( U(i) - \Delta U(i) \) is computed and compared with \( F(U(i)) \). If \( U(i) - \Delta U(i) \) results in an improvement, i.e., \( F(U(i) - \Delta U(i)) < F(U(i)) \), then \( U(i) - \Delta U(i) \) becomes the new base point. If the point \( U(i) - \Delta U(i) \) also fails to reduce the value of the objective functions, \( U(i) \) is maintained as the base point and \( \Delta U(i) \) is reduced to the value \( \Delta U(i) = \beta \cdot \Delta U(i) \), where \( \beta \) is defined by the user \( (0 < \beta < 1) \), and the search procedure is attempted with the new reduced \( \Delta U(i) \).
The effect of $\alpha$ and $\beta$ NOT shown.

FIGURE 3

TWO DIMENSIONAL EXAMPLE OF PATTERN SEARCH METHOD
If a success occurs at either $U(i) + \Delta U(i)$ or $U(i) - \Delta U(i)$, then $\Delta U(i)$ is increased to $\Delta U(i) = \alpha \cdot \Delta U(i)$, where $\alpha$ is specified by the user ($\alpha \geq 1$); thus, the search is accelerated in the $U(i)$ direction.

When an exploratory move lowers the performance function, i.e., a perturbation $U(i) + \Delta U(i)$, $i = 1, 2, \ldots, 24$ is a success, then the following procedure is used. Let $b_1$ specify the original base point at the start of the exploration procedure and let $b_2$ designate a new base point resulting from exploratory moves. The two base points establish a direction for a pattern move to a temporary head $t$. A pattern move is made in the direction specified by the vector direction $b_1$ to $b_2$ with a magnitude equal to twice the distance between $b_1$ and $b_2$ thus,

$$t = b_1 + 2(b_2 - b_1) = 2b_2 - b_1$$

At $t$, the exploration procedure is repeated. If an improvement occurs for an exploratory move from $t$, then a new base point $b_3$ is established and a new pattern direction, specified by $b_2$ to $b_3$ sets up a new temporary head

$$t = 2b_3 - b_2$$

This process is repeated until the value of the objective function is not reduced by all exploratory moves from a temporary head. At this time the pattern is destroyed and the entire process is restarted using the last base point as the starting value. A new set of exploratory moves is made from this base point to establish another base point for a pattern move. If the new set
of explorations does not establish a second base point, then the exploration moves are repeated using the reduced step size specified by \( \beta \). The process is repeated until either a new pattern is established or the steps in each independent variable are smaller than some preselected fraction of the original range of the variable.

Figure 3 is a graphical example of the following steps taken in a pattern search. Note that the effects of \( \alpha \) and \( \beta \) are not shown.

1. Base point \( b_2 \) established from exploratory moves originating from starting base point \( b_1 \).
2. Temporary head established by pattern move in direction from \( b_1 \) to \( b_2 \).
3. Base point 3 found as result of exploratory moves from \( t \).
4. New temporary head found by pattern moves from \( b_2 \) through \( b_3 \).
5. Base point 4 established from search initiated from \( t \).
6. Pattern move from \( b_3 \) through \( b_4 \) establishes temporary head \( t \).
7. Base point 5 located at \( t \) since function value after exploratory moves from \( t \) is less than value at previous base point 4.
8. Temporary head established by pattern move from \( b_4 \) through \( b_5 \).
9. Function values from exploratory moves at \( t \) not less than at base point 5; pattern is destroyed.
(10) Process restarted at base point 5 using new designation \( b_6 = b_5 \). New exploratory moves will *either* establish new pattern or reduce step sizes to within specified tolerances which will stop the search.

This method of optimization has been used successfully for the optimization of the Kraft Recovery Cycle. Example of results obtained, and copies of pertinent computer programs necessary will be found in the Report of Adler and Goodson (1).
PROPOSED DIGESTER CONTROL SYSTEM

There are three major types of changes or disturbances which occur in the Kamyr Digester that require dynamic compensation: First, there are required production rate and pulp quality changes. Except for emergencies, these are normally known well before hand as to the time and magnitude of the changes required. Second, there are uncontrollable but measureable disturbances to the feed conditions, such as the moisture content of the chips, density of the chips, concentration and sulfidity of the white liquor, etc. Third, there are operating and emergency changes that do not enter the system at the feed point. An example of this type of disturbances is an emergency change in production rate for maintenance of chip level.

Described below is a proposed control scheme to minimize the effects of these required changes and unexpected disturbances on the resultant pulp quality and production rate. In particular, compensation is especially made to maintain pulp quality constant even though the production rate may change due to slight changes in yield. Major variations in production rate can be compensated by a scheduled production rate change. The main element in the control system is an algebraic correlation between output variables and input variables of both control and disturbance type. This algebraic correlation is developed from the outputs of the dynamic model run repeated in an off-line mode varying the input variables. This has been done [1] for the case of steady state optimization.

The resultant form of the algebraic model is as follows:

\[ Y = Y_0 + BX \]
where \( Y = [Y_1, \ldots, Y_{18}]^T \), a vector of 18 output variables,
\[ Y_0 = [Y_{01}, \ldots, Y_{018}]^T \], a vector of constants,
\[ X = [X_1, \ldots, X_{14}]^T \], a vector of 14 input control and disturbance variables,
and \( B = (b_{ij}) \) a matrix of correlation coefficients relating inputs to outputs.

The elaboration of each variable is in Table III and the numbers for the \( Y_0 \) vector and \( B \) matrix are reported in [1].

Although all the controls are not used in the basic control scheme, the algebraic model is available for optimizing the settings of those other controls in regard to pulp cleanliness and maximum percent solids to the evaporators.

PULP QUALITY CHANGES

Changes in required pulp quality are achieved by a step change in the lower heater temperature controller set point.

\[ \Delta T_{LH_{SP}} = \frac{\Delta X_{pulp}}{b^{27}} \]  
(25)

This change is made \( t_R \) minutes prior to the required change at the blow line.

PRODUCTION RATE CHANGES

Scheduled production rate changes are achieved by a step change
TABLE III
ELABORATION OF CONTROLS, DISTURBANCES, AND OUTPUTS

<table>
<thead>
<tr>
<th>Controls and Disturbances (X)</th>
<th>Digester Outputs (Y)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1. CMRPM</td>
<td>1. Pulp production rate</td>
</tr>
<tr>
<td>2. $X_{OH}$ WL</td>
<td>2. Lignin as a fraction of pulp</td>
</tr>
<tr>
<td>3. Sulfidity of white liquor</td>
<td>3. $X_{pulp blow}$</td>
</tr>
<tr>
<td>$Na_2SO_4$ WL</td>
<td>4. Upper heater energy</td>
</tr>
<tr>
<td>5. $Na_2CO_3$ WL</td>
<td>5. Lower heater energy</td>
</tr>
<tr>
<td>7. Lower heater temperature</td>
<td>7. Upflow</td>
</tr>
<tr>
<td>controller set point</td>
<td></td>
</tr>
<tr>
<td>8. $W_{byp}$</td>
<td>8. Blow liquid (non pulp)flow</td>
</tr>
<tr>
<td></td>
<td>Solids concentration of blow liquid</td>
</tr>
<tr>
<td>9. $W_{blow}$</td>
<td>9. NaOH</td>
</tr>
<tr>
<td>10. Temperature of wash heater</td>
<td>10. NaSH</td>
</tr>
<tr>
<td>11. $W_{ext}$</td>
<td>11. Cellulose</td>
</tr>
<tr>
<td>12. $W_{WL}$</td>
<td>12. Lignin</td>
</tr>
<tr>
<td></td>
<td>Solids concentration of liquor to evaporator</td>
</tr>
<tr>
<td>13.* $X_{OH}$</td>
<td>13. NaOH</td>
</tr>
</tbody>
</table>
14.* $X_{SH}$

14. NaSH

15. Cellulose

16. Lignin

17. Liquor flow to evaporators

18. Net steam requirements to steaming vessel.

* Not included in correlation reported in [1].
in chip meter RPM, CMRPM. White liquor flow, $W_{WL}$, blow flow, $W_{blow}$, and temperature, $T_{LH_{SP}}$, are adjusted to maintain effective alkali/wood ratio, chip level, and pulp quality.

To achieve a desired production rate change

$$\Delta CMRPM = \frac{\Delta W_{pulp}}{b_{11}\rho_{BD}}$$  \hspace{1cm} (26a)

and to retain constant pulp quality

$$\Delta W_{WL} = \frac{CMRPM \times CMVOL \times \rho_{BD} \times EA/W}{X_{WL}}$$  \hspace{1cm} (26b)

$$\Delta W_{blow} = -\frac{b_{31}\Delta CMRPM}{b_{39}}$$  \hspace{1cm} (26c)

$$\Delta T_{LH_{SP}}(t) = -\frac{b_{21}\Delta CMRPM(t)}{b_{27}}$$  \hspace{1cm} (26d)

where the function of Equation (26d) is ramped as follows:

$$\Delta CMRPM(t) = \frac{\Delta CMRPM}{t_R} \times 0 < t < t_R$$

and $t_R$ is the time for instituting the new CMRPM.

At $t = t_R$, the required step changes to CMRPM, $W_{WL}$ and $W_{blow}$ should be made as stated in Equations (26a, b, c).

**MOISTURE COMPENSATION**

An increase in water addition with the chips will cause a dilution of the cooking liquor (liquid to wood ratio increase) and affect the resultant pulp. Thus the lower heater temperature set point will be adjusted to provide the same lignin/pulp ratio (proportional to $K$ number) for the dilution being caused by chip
moisture. Dilution water is chip moisture and steaming vessel condensate,

\[ W_{dil} = m \times W_{wd} + \frac{\left(C_{pwd} (1-m) + m\right) W_{wd} (T_{SV} - T_{amb})}{H_{SV}} \]  

(27a)

Therefore the chemical concentration being fed is:

\[ X_{OH} = \frac{X_{WL} W_{WL}}{W_{WL} + W_{dil}} \]  

(27b)

\[ X_{SH} = \frac{X_{WL} W_{WL}}{W_{WL} + W_{dil}} \]  

(27c)

A step change

\[ \Delta T_{IH} = \frac{-\left(b_{213} \Delta X_{OH} + b_{214} \Delta X_{SH}\right)}{b_{27}} \]  

(27d)

should be made to compensate for the change in dilution.

CHIP DENSITY COMPENSATION

A chip density change alters the relation between residence time and production rate; i.e., a decrease in chip density requires a higher volumetric feed rate and gives a lower residence time for a constant production rate. Thus a volumetric feed rate change calculated to maintain a constant dry wood feed rate, should be scheduled for the time the changed density reaches the blow line, i.e., the time of density change plus the old residence time.

\[ \Delta CMRPM = \left(\frac{\rho_{BD}}{\rho_{BD}^*} - 1\right) CMRPM \]  

(28)
The other corresponding changes are the same as for a production rate change.

WHITE LIQUOR CONCENTRATION COMPENSATION

Changes in white liquor concentrations either in effective alkali or sulfidity can be compensated for in exactly the same manner as changes in chip moisture content since both act to change the feed concentration of chemicals. First, however, white liquor flow is adjusted to maintain a constant effective alkali/wood ratio.

\[
\Delta W_{WL} = \left(\frac{X_{WL}^{OH}}{X_{WL}^{OH}} - 1\right) W_{WL}
\]

(29a)

\[
\Delta T_{LHSP} = -\left(\frac{b_{2,13} \Delta X_{OH} + b_{2,14} \Delta X_{SH}}{b_{27}}\right)
\]

(29b)

CHIP LEVEL MAINTENANCE

The blow flow is calculated so as to remove at the blow line the proper amount of pulp based on feed rate and expected yield.

\[
W_{blow} = \frac{CMRPM \times CMVOL \times \rho_{BD} \times \text{yield}}{X_{pulp}^{\text{pulp}}}
\]

(30a)

Should the chip level exceed the desired level a pulse in the blow flow of proper duration is calculated to alleviate the difference.

\[
T_{\text{blow pulse}} = \frac{\Delta \text{level} \times \rho_{BD} \times A_c \times \text{yield}}{\Delta W_{blow} \times X_{pulp}^{\text{pulp}}}
\]

(30b)
EMERGENCY FEED RATE CHANGES

Generally an emergency only involves a decrease in feed rate. Other parts of the process can wait for a scheduled increase. The effect of an emergency reduction is to increase the residence time beyond that which was expected and hence overcook the pulp. To compensate and to lose as little pulp as possible, an amount of cold filtrate (bypass) to be added to the quench circulation to reduce the temperature in the quench zone and a reduction in wash temperature to also reduce the wash zone temperature are calculated. The bypass addition is removed as the effects of the upflow cool the wash zone all the way to the quench zone. In addition an immediate move to set point values of \( W_{WL}, T_{LH}, \) and \( W_{blow} \) for the new feed rate is made.

\[
\Delta W_{\text{bypass}} = \frac{-b_{21}\Delta CMRPM}{b_{28}} \quad (31a)
\]
\[
\Delta T_{\text{wash}} = \frac{-b_{21}\Delta CMRPM}{b_{2,10}} \quad (31b)
\]
CONTROL OF WASH LIQUOR CONCENTRATION

To maintain a desired concentration of solids carried over with the pulp to the washers, the wash upflow, as influenced by the extraction flow, is maintained based on changes in dilution and white liquor flows given by Equations 27a and 29a. These are based on feed rate chip moisture, and white liquor active chemical concentration.

\[ \Delta W_{\text{ext}} = \Delta W_{\text{dil}} + \Delta W_{\text{WL}} + \Delta W_{\text{byp}} \]  

(32)

DESCRIPTION OF CONTROLLER

The controller thus consists of six elements which are the implementation of the relations developed by the algebraic model and the time delays as expressed in Equations (25 thru 32).

The pulp quality controller is responsible for the maintenance of a constant lignin/pulp ratio (proportional to K No.). It is influenced by the volumetric feed rate and white liquor active chemical concentrations. It computes a lower heater set point, white liquor flow, and steady-state blow flow (Equations 25, 26 b, c, d, 29, and 30a) to achieve the desired results.

The moisture compensator acts in addition to the pulp quality controller to adjust the lower heater temperature set point based on the variable moisture dilution of the chemicals fed (Equations 27a - d) to maintain the lignin/pulp ratio.

The chip density compensator and production rate controller define the required volumetric feed rate based on chip density and
required pulp production rate. (Equations 26a and 28)

The level controller pulses the blow line flow (Equation 30b) to maintain a constant level.

The wash controller acts to maintain solids carry-over with the pulp constant by manipulating the extraction flow to maintain the wash upflow. (Equation 32).

Although all production rate changes are normally planned well in advance, plant upsets may cause a dynamic change in the called for production rate to the production rate controller. In the case of such unplanned (emergency) changes the dynamic production rate controller and pulp quality controller attempt to maintain pulp quality by adjusting bypass flow and wash temperature. (Equations 31a, b)

Figure 4 diagrams the resulting total control system while Table III summarizes the controls used, the disturbances encountered and the outputs involved. Symbols used in this part of this Section are listed with Section IV.
FIGURE 4

DIAGRAM OF PROPOSED DIGESTER CONTROL SYSTEM

Desired SS solids
Carry-over to washers

WASH CONTROLLER

MOISTURE CONTENT COMPENSATION

PULP QUALITY CONTROLLER

LEVEL CONTROLLER

CHIP DENSITY COMPENSATOR AND PRODUCTION RATE CONTROLLER

DYNAMIC PRODUCTION RATE DETERMINATION

PLANT UPSET AND CAPACITY INPUTS

Desired Steady-state Production Rate

desired Steady-state Production Rate

Carry-over to washers

required Delignification (K Number)

chip density compensator and production rate controller

Dynamic production rate determination

Plant upset and capacity inputs

Desired SS solids

Chip level indication

CMRPM

$\Delta W_{\text{blow}}$

$T_{\text{LHSP}}$

$W_{\text{bypass}}$

$W_{\text{WL}}$

$W_{\text{ext}}$

$X_{\text{OHWL}}$

$X_{\text{SHWL}}$

$\rho_{\text{BD}}$

$\frac{m}{W}$

$W_{\text{WL}}$

$W_{\text{WL}}$

$W_{\text{WL}}$
THE MULTI-EFFECT EVAPORATOR CONTROL SCHEME

In general, a multi-effect evaporator operates under one of two distinct conditions:

1. Full capacity, i.e., all the steam available is supplied to the evaporator system, and the mass flow rate of the weak black liquor fed to the Fifth and Sixth Effects is varied to maintain the concentration of strong black liquor coming out of First Effect at some predesignated value.

2. The mass flow rate of weak black liquor is limited (i.e., the evaporators are operating at less than their maximum capacity), and thus steam flow rate to the First Effect can be varied to maintain the concentration of strong black liquor coming out of the First Effect at some desired value.

The two control schemes, as shown in Figure 5, and Figure 6, were devised to take care of either of these operating conditions. In the first, the mass flow rate of weak black liquor is varied to take care of disturbances in the concentration of weak black liquor and in the available mass flow rate of steam. In the second, the mass flow rate of steam is varied to take care of disturbances in both the mass flow rate and the concentration of weak black liquor.

The development and adjustment of the control schemes was guided by a criterion, that a good control scheme should be able to maintain the strong black liquor concentration within $51.4\% \pm 0.3\%$ ($51.4\%$ is the operating point) for a $2\%$ (i.e., $15\%$ to $17\%$)
FIGURE 5
CONTROL SCHEME 1
STEAM LIMITED CASE

Flow Sensor

Weak Black Liquor

Conc. Sensor

Multi Effect Black Liquor Evaporators

P.I. Controller

Primary Steam

Strong Black Liquor

FFR

Feedforward Controller
FIGURE 6
CONTROL SCHEME 2
WEAK BLACK LIQUOR LIMITED CASE
step disturbance in weak black liquor concentration and for similar sized disturbances in steam flow rate in the first scheme, and in weak black liquor flow rate in the second scheme. For the size of disturbances considered, the requirements of a control scheme are far more stringent than those in use in industry at the present time. However, it is felt that these requirements will allow a substantially reduced inventory of weak black liquor, and a more efficient operation of the multi-effect evaporator system.

The accurate control of these units as described here should also decrease entrainment due to surges in the system but has no way of detecting or correcting for some other sources of inefficient evaporator operation such as entrainment.

It was found that for the range of disturbances under consideration, a conventional PI feedback controller could not maintain the strong black liquor concentration within the specified range during the transient period. Therefore, the control schemes proposed include both a dynamic feedforward controller (which takes into account the dynamics of the evaporators and compensates for them before the disturbances substantially affect the strong black liquor concentration) and a PI feedback controller (which takes care of slow variations in the feed temperature and in the vacuum level maintained by a condenser in the last effect, and of errors due to non-linearities inherent in the system).

STEADY-STATE EQUATIONS FOR FEEDFORWARD CONTROLLERS

Since small variations in feed temperature and in condenser vacuum can be taken care of by a feedback PI controller, the strong
black liquor concentration, $C_{BLO1}$, can be considered as a function of mass flow rate of weak black liquor, $\dot{M}_{WBL}$, concentration of weak black liquor, $C_{WBL}$, and mass flow rate of steam, $\dot{M}_{HSTCH1}$. That is,

$$C_{BLO1} = f(\dot{M}_{WBL}, C_{WBL}, \dot{M}_{HSTCH1}) \quad (33)$$

For small changes about the operating point, i.e., $\Delta\dot{M}_{WBLSS}$, $\Delta C_{WBLSS}$ and $\Delta\dot{M}_{HSTCH1SS}$ in $\dot{M}_{WBL}$, $C_{WBL}$, and $\dot{M}_{HSTCH1}$ respectively, the steady-state change $\Delta C_{BLO1SS}$ in $C_{BLO1}$ can be expressed in a linear form about its own operating point as:

$$\Delta C_{BLO1SS} = \frac{\partial C_{BLO1}}{\partial \dot{M}_{WBL}} \Delta \dot{M}_{WBLSS} + \frac{\partial C_{BLO1}}{\partial C_{WBL}} \Delta C_{WBLSS} + \frac{\partial C_{BLO1}}{\partial \dot{M}_{HSTCH1}} \Delta \dot{M}_{HSTCH1SS} \quad (34)$$

The steady-state concentration of strong black liquor must remain unchanged for a perfect steady-state control. Therefore:

$$\Delta C_{BLO1SS} = 0 \quad (35)$$

Thus Equation (34) can be written as

$$A \Delta \dot{M}_{WBLSS} + B \Delta C_{WBLSS} + C \Delta \dot{M}_{HSTCH1SS} = 0 \quad (36)$$

where $A$, $B$, and $C$ are coefficients of the corresponding terms in Equation (34) evaluated at the operating point. In another words, $A$, $B$, and $C$ are the ratios of the change in strong black liquor concentration due to changes in turn to weak black liquor mass flow.
rate, weak black liquor concentration, and to steam mass flow rate.

Coefficients A, B, and C of Equation (36), which are also parameters of the feedforward controller can be determined either from the simulation of the linear dynamic model of Section V on a computer, or by solving the system of steady-state mass and energy balance equations on a digital computer (in theory, they can also be solved analytically). For the example of the controller schemes given in this report, the controller parameters A, B, and C were obtained from simulations of all six effects on the hybrid computer. This was achieved by introducing step changes, first, in mass flow rate of weak black liquor only, second in concentration of weak black liquor only, and third, in mass flow rate of primary steam only, and then recording the response of strong black liquor concentration due to these disturbances. Figure 7 presents an example of such a simulation in this case, the variation of $\Delta C_{BLO}$ with $\Delta C_{WBL}$. For this linear approximation it is not necessary to include terms involving higher powers of the disturbances or interactions involving products of the disturbances.

The ratios, A, B, and C, are then determined from the new steady-state concentration values of these simulations as follows:

From Figure 7 and similarly: $A = \frac{\Delta C_{BLO1SS}}{\Delta M_{WBL}}$

$B = \frac{\Delta C_{BLO1SS}}{\Delta C_{WBL}}$

$C = \frac{\Delta C_{BLO1SS}}{\Delta M_{HSTCH1}}$
\[ \Delta \dot{m}_{WBL} = 10000 \text{ lbs/hr} \]

\[ \Delta \dot{m}_{HSTCH 1} = 4000 \text{ lbs/hr} \]

**FIGURE 7**

DETERMINATION OF SENSITIVITY COEFFICIENTS A, B, AND C FROM HYBRID COMPUTER SIMULATIONS
The feedforward controller in Control Scheme 1 alters the weak black liquor mass flow rate such that it immediately cancels out the contributions due to disturbances in weak black liquor concentration, and in steam flow rate under steady-state conditions. Similarly, the steam mass flow rate takes care of the two remaining disturbances in Control Scheme 2.

CONFIGURATION OF DYNAMIC FEEDFORWARD CONTROLLERS

Steady-state equations for feedforward controllers were derived in the previous part. However, the actual configuration of the feedforward controllers, which are dynamic in nature, is more complex than appears from Equation (36), because they must also maintain the concentration of strong black liquor within a narrow range during the transient periods of operation. The dynamics of the evaporators is obtained from simulations of the linear dynamic mathematical model given in Section V on the hybrid computer. It was seen from these graphical results that the response of $\Delta C_{BL01}$ due to a step change, $\Delta M_{WBL}$, as given in Figure 7A, can be approximated by the transfer function, $T_1(s)$, as,

$$T_1(s) = \frac{\Delta C_{BL01}}{\Delta M_{WBL}} = -p_1 - \frac{p_2 \ e^{-p_3(s)}}{p_4 s + 1}$$

(37)

where $p_1$, $p_2$, $p_3$, and $p_4$ are positive constants developed for small variations about an operating point. It may be noted that at steady-state the Laplace variable $s$, approaches zero, and therefore,

$$A = \frac{\Delta C_{BL01}}{\Delta M_{WBL}} = -(p_1 + p_2)$$

(38)
The response for $\Delta C_{\text{BLOl}}$ due to a step change $\Delta C_{\text{WBL}}$, as given in Figure 7B, can be approximated by transfer function, $T_2(s)$, as

$$T_2(s) = \frac{\Delta C_{\text{BLOl}}}{\Delta C_{\text{WBL}}} = \frac{-q_1}{q_2 s + 1} + \frac{q_3 e^{-q_4 s}}{q_5 s + 1} \quad (39)$$

Here $q_1$, $q_2$, $q_3$, and $q_4$ are again positive constants specific for a particular operating point. Among these $q_2$ is a larger time constant than $q_5$. At steady-state the transient terms disappear and

$$B = \frac{\Delta C_{\text{BLOl}}}{\Delta C_{\text{WBL}}} = -q_1 + q_3 \quad (40)$$

The response for $\Delta C_{\text{BLOl}}$ due to a step change $\Delta M_{\text{HSTCH1}}$, as given in Figure 7C, can be approximated by the transfer function, $T_3(s)$, as,

$$T_3(s) = \frac{\Delta C_{\text{BLOl}}}{\Delta M_{\text{HSTCH1}}} = \frac{Y_1}{Y_2 s + 1} + \frac{Y_3 e^{-Y_4 s}}{Y_5 s + 1} \quad (41)$$

where $Y_1$, $Y_2$, $Y_3$, $Y_4$, and $Y_5$ are again positive constants, and $Y_2$ is a smaller time constant than $Y_5$. At steady-state,

$$C = \frac{\Delta C_{\text{BLOl}}}{\Delta M_{\text{HSTCH1}}} = Y_1 + Y_3 \quad (42)$$

**FEEDFORWARD CONTROLLER - SCHEME 1**

Under this control scheme, the dynamic feedforward controller varies the mass flow rate of weak black liquor such that it compensates for the effect of disturbances in concentration of weak black liquor and in the mass flow rate of available steam. Therefore,
for the control

\[ \Delta C_{BLO1} \text{ due to } \Delta \dot M_{WBL} = ( - \Delta C_{BLO1} \text{ due to } \Delta C_{WBL} ) + ( - \Delta C_{BLO1} \text{ due to } \Delta \dot M_{HSTCH1} ) \] (43)

or,

\[ T_1(s) \Delta \dot M_{WBL} = - T_2(s) \Delta C_{WBL} - T_3(s) \Delta \dot M_{HSTCH1} \] (44)

or,

\[ \Delta \dot M_{WBL} = - \frac{T_2(s)}{T_1(s)} \Delta C_{WBL} - \frac{T_3(s)}{T_1(s)} \Delta \dot M_{HSTCH1} \] (45)

Let \( T_4'(s) \) be defined as

\[ T_4'(s) = - \frac{T_3(s)}{T_1(s)} = \frac{\frac{\gamma_1}{s + 1} + \frac{\gamma_3}{s + 1} e^{-\gamma_4 s}}{\frac{\gamma_2}{s + 1} + \frac{\gamma_5}{s + 1} + \frac{p_2 e^{-p_3 s}}{p_1 + \frac{p_4}{s + 1}}} \] (46)

The transfer function \( T_4'(s) \) can be approximated by \( T_4(s) \) given by

\[ T_4(s) = \frac{t_1 (t_2 s + 1)}{t_3 s + 1} \] (47)

where \( t_1 = C/A \).

Equation (45) can now be written as,

\[ \Delta \dot M_{WBL} = - \frac{T_2(s)}{T_1(s)} \Delta C_{WBL} + T_4(s) \Delta \dot M_{HSTCH1} \] (48)

This equation in conjunction with Equations (37), (39), and (47) describes the dynamic feedforward controller for Control Scheme 1. The configuration of the controller is given in Figure 8. It may be observed that the feedforward controller contains blocks which depend on the dynamic response of
NOTE: \( \ldots \) represents S. S. value at an operating point

FIGURE 8

CONFIGURATION OF FEEDFORWARD CONTROLLER

SCHEME 1
the evaporator to changes in the concentration of weak black liquor, the mass flow rate of weak black liquor, and the mass flow rate of steam. Therefore, in a case where the actual response of the multi-effect evaporator to some specific disturbance differs from the one obtained from the linear dynamic model, only the block describing that response needs modifications.

FEEDFORWARD CONTROLLER - SCHEME 2

Under this second control scheme, the dynamic feedforward controller varies the mass flow rate of steam such that it compensates for the effect of disturbances in concentration and mass flow rate of weak black liquor. Thus, for the control

\[ \Delta C_{BL01} \text{ due to } \Delta M_{HSTCH1} = (- \Delta C_{BL01} \text{ due to } \Delta M_{WBL}) + \]

\[ (- \Delta C_{BL01} \text{ due to } \Delta C_{WBL}) \]

(49)

This equation can be written, using Equations (37), (39), (41), (46) and (47), as,

\[ \Delta M_{HSTCH1} = \frac{1}{T_4(s)} \left[ \Delta M_{WBL} - \frac{T_2(s)T_4(s)}{T_3(s)} \Delta C_{WBL} \right] \]

(50)

\[ = \frac{1}{T_4(s)} \left[ \Delta M_{WBL} - \frac{T_2(s)}{T_5(s)} \Delta C_{WBL} \right] \]

(51)

where \( T_4(s) = \frac{T_3(s)}{T_4(s)} \) is approximately described by

\[ T_5(s) = u_1 + \frac{u_2 e^{-u_3 s}}{u_4 s + 1} \]

(52)
Here, \( u(1), u(2), u(3), \) and \( u(4) \) are positive constants (with \( u(1) + u(2) = c \)) at an operating point.

Equation (51) in conjunction with Equations (39), (47), and (52) describes the dynamic feedforward controller for Control Scheme 2. The configuration of the controller is given in Figure 9.

RESULTS FROM TEST SIMULATIONS OF THE PROPOSED CONTROL SCHEMES

For a demonstration of the effectiveness of the dynamic control schemes presented here, results of ten simulations are presented. Three of these show the effect on strong black liquor outlet concentration due to a 1% (15% to 16%) step change in weak black liquor concentration under the following conditions:

1. When no control action is taken (Figure 10).
2. When only a steady-state feedforward controller is used (Figure 11).
3. When both the dynamic feedforward controller and the feedback PI controller of Scheme 1 are used (Figure 12).

The following comments concerning the results obtained may be worth noting:

1. Figure 10, shows the variation of strong black liquor concentration with no control action being taken. The initial drop in strong black liquor concentration occurs due to changes in boiling point in all six effects.
2. Figure 11, shows the response of a steady-state feedforward controller to a step disturbance in weak black liquor
NOTE: ... represents S.S. value at an operating point

FIGURE 9
CONFIGURATION OF FEEDFORWARD CONTROLLER
SCHEME 2
FIGURE 10

RESPONSE OF EVAPORATOR SYSTEM TO A $C_{\text{WBL}}$ DISTURBANCE,

WHEN NO CONTROL ACTION IS TAKEN.
RESPONSE OF SYSTEM WITH STEADY-STATE FEED FORWARD CONTROLLER ON WEAK BLACK LIQUOR TO A DISTURBANCE IN $C_{WBL}$
concentration. This result occurs, because the steady-state feedforward controller changes the weak black liquor flow rate instantaneously, as shown in Figure 11.

3. Figure 12, shows the increases in mass flow rate due to the feedback (PI) controller, and dynamic feedforward controller respectively.

As expected the steady-state concentration of strong black liquor is reached with a mass flow rate 8000 lbs/hr above its initial steady-state value of 334,000 lbs/hr for both the steady-state feedforward schemes (Figure 11), and (Figure 12). However, the dynamic feedforward controller varies the mass flow rate of weak black liquor over approximately twice the range of the steady-state correction to compensate for evaporator dynamics thereby maintaining the strong black liquor concentration within a very small range during the transient period. The dynamic feedforward control along with the feedback PI controllers are able to jointly maintain the concentration within 51.4 ± 0.15% for a 1% (15% to 16%) step change in weak black liquor concentration (Figure 12). The result substantially differs with that for a manual or a steady-state feedforward controller (used by industry at the present time), which leave an uncompensated transient deviation of approximately 2.9% in strong black liquor concentration for an equal disturbance in concentration of weak black liquor (Figure 11).

The effectiveness of Control Scheme 2 is demonstrated by the following simulated responses of the controlled system for:

1. Dynamic feedforward and PI feedback controllers with a disturbance in $C_{WBL}$ (Figure 13)
2. Dynamic feedforward and PI feedback controllers with a disturbance in $\dot{M}_{WBL}$ (Figure 14)
FIGURE 13
RESPONSE OF SYSTEM WITH DYNAMIC FEED FORWARD
AND PI FEEDBACK CONTROLLERS ON STEAM TO A $c_{wbl}$ DISTURBANCE (CONTROL SCHEME 2)
Figure 14

Response of system with dynamic feed forward and PI feedback controllers on steam to a \( M_{WBL} \) disturbance (control scheme 2)
3. Steady-state feedforward controller with a disturbance in \( C_{WBL} \) (Figure 15A)

4. Steady-state feedforward controller with a disturbance in \( \dot{M}_{WBL} \) (Figure 15C)

Figure 13 shows that the proposed control Scheme 2 can maintain the concentration of strong black liquor at outlet within \( 51.4 \pm 0.1\% \) for a disturbance of 1\% in concentration. On the other hand, the results for a steady-state controller range between 51.47 and 47.9\% for the same amplitude of disturbance in \( C_{WBL} \). Similar results are obtained for a disturbance in \( \dot{M}_{WBL} \) as shown by Figures 14 and 15C.

To show that a conventional PI controller can not meet the requirements imposed on the control scheme, three responses are given of the system with a PI feedback controller alone;

1. On weak black liquor for a disturbance in \( C_{WBL} \) (Figure 6)
2. On steam for a disturbance in \( C_{WBL} \) (Figure 17A)
3. On steam for a disturbance in \( \dot{M}_{WBL} \) (Figure 17C)

For a 1\% (15\% - 16\%) step disturbance in weak black liquor concentration a conventional PI controller on weak black liquor can maintain strong black liquor outlet concentration between 51.2 and 52.75\% (Figure 16) in contrast with 51.4 \pm 0.15\% for the proposed Control Scheme 1 (Figure 12). For the same disturbance in weak black liquor concentration a conventional PI controller on steam can maintain strong black liquor outlet concentration within 51.35 - 52.95\% (Figure 17A) in contrast with 51.4 \pm 0.10\% for the proposed Control Scheme 2 (Figure 13). The similar results are
FIGURE 16

RESPONSE OF SYSTEM WITH PI FEEDBACK CONTROLLER ON WEAK BLACK LIQUOR TO A DISTURBANCE IN C_{WBL}
FIGURE 17
RESPONSE OF SYSTEM WITH PI FEEDBACK CONTROLLER
ON STEAM TO DISTURBANCES IN $c_{WBL}$ AND $m_{WBL}$
obtained for a disturbance in flow rate of weak black liquor as shown in Figures 14 and 17C.

Thus it is seen that the proposed control schemes appear to be a substantial improvement over the conventional control schemes in use in industry at the present time.

MEASUREMENTS NECESSARY

Following measurements are required for a good steady-state and dynamic control system.

1. Mass flow rate, concentration, and temperature of weak black liquor,
2. Mass flow rate, concentration, and temperature of strong black liquor,
3. Mass flow rate of steam,
4. Pressure and temperature in the steam-chest of Effect 1,
5. Vacuum in the vapor space of final effect,
6. Temperatures of black liquor leaving Effects 2, 3, 4, 5, and 6,
7. Either the temperatures in steam-chests for Effects No. 2, 3, 4, 5 and 6 (or pressures of vapor spaces for Effects No. 1, 2, 3, 4 and 5).

In actual practice both Scheme 1 and Scheme 2 would be programmed in the advanced control section of the dual dynamic control computers. Then the appropriate one of the two would be selected to make the appropriate correction to the particular upset condition which existed at that moment.
The temperatures and flows from the various units, together with the appropriate energy balance, could, of course, be used for such additional and useful tasks as monitoring the fouling of the heat exchange tubes and giving an indication as to when cleaning or boil-out should be performed.
PROPOSED DIGITAL CONTROL SYSTEM FOR THE RECOVERY FURNACE

INTRODUCTION

The purpose of the proposed digital control system is to maintain operation at a maximum degree of efficiency and also to improve safety by eliminating the need for the continuous presence of the operating personnel at the furnace.

The main control duties of the operator are to maintain a proper char bed level, a good fire, and a correct primary air deficiency in the furnace. It is suggested that these duties be taken over by the proposed char bed level control and combustion air control system.

A method for the automatic detection of air port plugging is proposed and the possibility of a useful automatic cleaning system is suggested. The continual manual cleaning of the air ports is perhaps the one operation which is most resistant to automation and the subsequent decrease in hazards to the people performing this operation.

Replacement of conventional analog controllers with D. D. C. for the several minor control loops in the recovery unit is also considered.

In order to operate the furnace at the best operating point one should use the following criteria:

1. Keep the primary air flow low in order to produce a high smelt reduction ratio.

2. Use a heavy spray, but avoid quenching the fire in the char bed.
3. Maintain the proper total air flow and uniform secondary zone turbulence by adjusting the secondary air flow and the windport dampers. All these conditions can be fulfilled simultaneously, and hence there seems to be no need for a complicated search for an optimum operating point.

The above arguments were based upon liquor of constant flow and composition to the spray nozzles. Since the water content of the black liquor coming from the cascade evaporator does vary and since these variations affect mainly the char bed height, the next part of this Section concerns the spray action, its control, and its effect upon the char bed level in the furnace.

PROPOSED CHAR BED LEVEL INSTRUMENTATION AND CONTROL SYSTEM

Figure 18 shows a diagram of the **proposed** char bed level control system. The object here is to develop a system that can automate the present hazardous duties of the operator and his helper. A reliable automatic level measuring system is required, and to the knowledge of the author no system capable of operating at these temperatures is presently being used. It does seem feasible to devise a crude system which can determine whether the char bed level is above or below a certain prefixed point. Such a system might make use of a strong light source and a photosensitive detector. The light source and the detector can be mounted in openings in opposite facing furnace walls such that the light beam will have to cross the center of the combustion chamber.

As both the gases and the char bed emit light, there will be
FIGURE 18
PROPOSED CHAR BED LEVEL CONTROL SYSTEM
need for a strong light source preferable with wavelengths different from the wavelengths of the major energy emissions from the gas and the char bed. The light source could be modulated with a periodic signal (square wave or sinusoid) in order to decrease the effect of disturbances from the combustion chamber. The light source could be a laser with the appropriate wavelength.

The proposed system will require some modifications to be made to the furnace walls. It is not possible to simply punch holes in the walls, as the inside of each wall is covered with closely spaced water tubes. The viewports must also be kept clean from smelt flowing down the walls, possibly by a system of steam nozzles that would blow off the solidified smelt at regular intervals.

Some experimenting will probably have to be done in order to find the best location for the light beam. It may be that a trajectory slightly off center will be less subject to disturbances from flames than the one proposed. For cases of strong interference more than one light beam could be used.

Alternative systems that can sense the position of the char bed from the radiation emitted inside the combustion chamber may possibly be designed, but so far there does not appear to be any practical solutions available.

At the present time, with the effect of the char bed level on the reduction ratio uncertain, it appears that a char bed level control system that can maintain the char bed level in the neighborhood of a certain prefixed level will be satisfactory. In this case a control system may be designed on the basis of the proposed
level sensing system. A cycling situation is purposely designed such that the char bed level will oscillate a small amount about the prefixed level. The amplitudes and the period of the oscillation are determined by the value of the gain, \( K_{cl} \), the limit temperatures, \( T_{lhi} \) and \( T_{llo} \), the resolution of the level sensor, and the combustion rate on the char bed surface.

Some experimentation will be required in order to find the best values of the controller parameters. When a set has been found, however, they are not expected to need frequent adjustment, as the present manual control practice requires only a very few and quite small changes in the liquor temperature.

In Figure 19 a simplified computer program flow diagram for the box labelled "limit adjustment" in Figure 18 is shown. The purpose of the "limit adjustment" is to adjust the limits, \( T_{llo} \) and \( T_{lhi} \), if the char bed level does not respond to the normal control action within a certain period of time, \( t_{per} \). This happens if a major disturbance in the inputs to the furnace occurs. The magnitude of the temperature band, defined as \( \Delta T_{li} = T_{lhi} - T_{llo} \), is kept constant at all times. The temperature increment, \( \Delta T_{lst} \), must be determined experimentally.

At a spray temperature which is too low the spray pattern disappears, and the liquor leaves the nozzles as a rope (roping). This condition will quickly quench the fire in the char bed and cause a black out. If the computed \( T_{llo} \) is too close to the roping temperature the old value should be retained and an alarm should be given. \( T_{blmn} \) is used as a preset lower temperature limit.

As will be commented on later in this Part, the best
FIGURE 19
SIMPLIFIED FLOW DIAGRAM FOR "LIMIT ADJUSTMENT"
operation of the furnace is achieved by using the heaviest liquor spray possible. Accordingly, the safety margin to the roping temperature should not be too large.

The control system should have the ability to compensate for the effects of major changes in the liquor properties that might require large parameter adjustments.

Even without roping, the char bed may black out when the liquor temperature is low and the resulting spray pattern consists mainly of large droplets.

It therefore seems necessary to require automatic sensing of the char bed surface temperature in order to protect against a black out situation. This sensing may be accomplished by a radiation pyrometer. In order to cover most of the char bed surface, two or more pyrometers could be used, or an oscillating prism could be used. Compensation for changes in surface emissivity is obtained by using two-color or two-wavelength pyrometers.

The flow diagram in Figure 20 shows how the temperature monitoring system interacts with the char bed level control system. A minimum char bed surface temperature $T_{cmin}$ must be specified. The temperature monitoring system has the ability to override the normal action of the level control system, and functions as follows (see Figure 20):

1. The char bed surface temperature is read off frequently, and in case it is too low, an alarm will be given.

2. The liquor temperature $T_{bl}$ and the two temperature limits, $T_{lhi}$ and $T_{llo}$, are all increased the same amount $\Delta T_{bl}$. 
FIGURE 20
FLOW DIAGRAM FOR CHAR BED TEMPERATURE MONITORING SYSTEM
4. The resulting liquor temperature is checked against a preset limit to guard against unforeseen problems. This is necessary as more than one liquor temperature increase may be required.

5. The spray temperature is kept constant during the time period, $t_{\text{delay}}$, while the char bed temperature is monitored. $t_{\text{delay}}$ should be quite short, - only a few seconds.

6.-7. If the char bed temperature increases, then once it has risen above $T_{\text{cmin}}$, the normal level control system can take over, using the new limits, $T_{\text{hi}}$ and $T_{\text{lo}}$. If no increase takes place, then a further step increase in liquor temperature should be called for and the sequence is repeated from Point 3.

The main task of the temperature monitoring system is therefore to prevent a too-low liquor temperature from creating a black out.

Safety is extremely important in a control system of this type. If for some reason the light beam is deflected or blocked by other means than the char bed, the situation will be interpreted as a high char bed and the liquor temperature will be increased. If the situation persists, then the char bed will burn down and excessive carryover will be generated. Prolonged operation in this manner may damage the furnace bottom. However, if the computer is programmed to check for a maximum time limit on the period of the char bed level cycle, then the situation can be detected automatically and relatively quickly. Thus the possibility of permanent
damage is reduced.

If the field of the pyrometers is blocked by solidified smelt, then the readings will be low. (Some of the more typical errors can be detected by preprogrammed error checking routines). A low char bed temperature will call for an increase in spray temperature. This will eventually burn the char bed down, cause an alarm, and overrun the time limit on the period of the level cycle.

Two situations must be prevented by reliable design methods:
1. The possibility of interpreting a high char bed as a low reading, since this will result in the blocking of primary air ports.
2. An erroneous, too high, pyrometer reading which may prevent the temperature monitoring system from detecting a black out.

The proposed level sensing system is very crude. A simple improvement can be made by adding one or more light beams at different levels and modify the control system accordingly. However, these systems will not be discussed further in the present study as a single light beam gave satisfactory control during the simulations.

PROPOSED COMBUSTION AIR CONTROL SYSTEM

Figure 21 shows a diagram of the proposed combustion air control system. The main differences between this system and the present control system are:

1. The primary combustion air is automatically adjusted so that the furnace will operate with as heavy liquor spray
FIGURE 21

PROPOSED COMBUSTION AIR CONTROL SYSTEM
as possible. This is accomplished by the block "Automatic Gain Adjustment" in Figure 21.

The advantage of operating with a heavy spray is that there will be less entrainment of the liquor droplets. A decrease in the entrainment will also cause a decrease in the flow of carbonate and salt cake in the black liquor recycling from the precipitator and the cascade evaporator. The black liquor solids from the spray nozzles will consist only of input solids and salt cake makeup. The char bed will have the same composition as the black liquor solids.

A small entrainment will carry less sulfur to the secondary zone and the generation rate of sulfurous gases will decrease. Less solids will be available to form deposits on the heat transfer surfaces, and the emission of particulates from the precipitator will be reduced.

2. A feedforward control system adjusts the primary and secondary air flows in proportion to the flow of input solids in the black liquor to the furnace, not just in proportion to the total flow of black liquor.

The concentration of input solids alone may be difficult to measure at this point (between the black liquor heater and the spray nozzles) due to the presence of salt cake and sodium carbonate precipitate. The salt cake makeup is known and can be compensated for. The usual refractive-index sensors are believed to measure the total solids...
concentration, and they must therefore be compensated by some other means. If the viscosity of the black liquor were less sensitive to salt cake and carbonate than to input solids, then the motor current to the cascade evaporator might be used as a measure of the input solids concentration.

An alternative method is shown in Figure 22. The concentration of input solids and the liquor flow could be measured at the black liquor input to the precipitator bottom. At this point there will be no errors in the measurement of the input solids concentration due to salt cake and sodium carbonate. To compensate for the effect of the precipitator bottom and the cascade evaporator vat, a corresponding dynamic correction could be applied to the signal from the solids meter.

Known changes in the heat value of input solids caused by variations in the ratio between organics and inorganics can be compensated for.

3. A feedback signal from the oxygen analyzer in the flue gas duct is used to correct the feedforward computation of total combustion air. Automatic adjustment of the windbox dampers maintains the desired degree of turbulence in the secondary zone.

In Figure 21 the primary signals from the sensors are multiplied together and then filtered. The dynamic filter compensates for both lag and delay in the process between a change in the input
FIGURE 22

ALTERNATIVE MEASUREMENT OF INPUT SOLIDS FLOW TO FURNACE
solids flow and the resulting change in the combustion rate in the char bed.

Filter 1 is a simple averaging filter.

\[
(w_{\text{bls}})_n + 1 = (1-a) (w_{\text{bls}})_n + a(w_{\text{bls}})_n + (sp)^n \text{X}(sp)_n
\]  

\[0 \leq a \leq 1\]

The "higher heat value" flow, \(w_h\), to the furnace is then computed as

\[w_h = w_{\text{bls}} H_{\text{bls}}\]

where \(H_{bls}\) is the higher heat value of input solids. When the ratio of organics to inorganics changes the value of \(H_{bls}\) should be adjusted accordingly.

The feedforward computation of total air flow is

\[w_{\text{atff}} = w_h K_{at}\]

where \(K_{at}\) is a constant coefficient, adjusted to give the furnace the correct amount of total air.

The set point to the total air flow controller is computed as

\[w_{ats} = w_{\text{atff}} - \left(\frac{w_{1a} + w_{2a}}{2}\right) + \Delta w_{O_2a}\]

where the primary and secondary infiltration air are subtracted from the feedforward computed total air. A feedback signal from the oxygen analyzer, \(\Delta w_{O_2a}\), has been added to correct for inaccuracies in the feedforward computation.
The air flow controller adjusts the vanes of the forced draft fan.

The feedforward computation of primary air flow set point is

\[ w_{as}^{(1)} = w_h K_{al} - w_{ia}^{(1)} \]  (57)

where \( K_{al} \) is a coefficient which is automatically adjusted online. The functions of the automatic gain adjustment will be described later in this section. The flow of primary infiltration air has been subtracted, yielding \( w_{as}^{(1)} \) as the primary air flow to be supplied by the combustion air system. The primary air flow controller adjusts the vanes in the primary air duct.

Adjustment of the secondary air port dampers is accomplished by the computation of the required air port area as a function of secondary air flow in order to keep the air velocity into the furnace constant.

\[ A_{po}^{(2)} = K_{po} \left[ w_{ats} - w_{as}^{(1)} \right] \]  (58)

A motor driven arrangement is required to implement Equation (58).

The purpose of the automatic gain adjustment for the primary air flow computation is to force the char bed level control system to use as heavy a spray as possible. Although the furnace can be operated with a wide variety of primary air-liquor spray temperature combinations, the best smelt reduction ratio is obtained when the spray temperature is as low as possible, causing a minimum amount of entrainment. The absolute lower limit on the spray temperature is the "roping" temperature, at which the spray pattern is lost. In practice one should go as close to the roping temperature as can be considered safe.
At an operating point with a non minimum spray temperature there will be recycling of salt cake and sodium carbonate in the liquor, and there will also be a corresponding amount of salt cake and carbonate in the reacting char in the char bed.

To decrease the recycle of salt cake and carbonate the entrainment must be reduced. This is accomplished by reducing the liquor temperature. At the same time the primary air flow must be increased to compensate for the evaporation of the additional water from the black liquor. If this were not done, the char bed level would increase due to both the cooling of the char bed and the increased liquor flow. The increase in primary air will cause the reduction ratio to drop immediately. The reduction ratio will be low as long as the spray temperature is being decreased. However, as soon as the minimum spray temperature has been reached the reduction ratio will slowly improve until it finally is often higher than it was initially.

Unfortunately due to the large time constants associated with the liquor volumes in the precipitator and the cascade evaporator vat (time constants of approximately one hour each) it takes a long time to build up the input solids concentration in the char bed. It would clearly be an advantage to collect the precipitates separately and add them to the liquor in a small volume just before the entering of the liquor to the furnace.

In order to have an acceptable smelt reduction ratio in the transient period while the liquor temperature is being reduced, the coefficient $K_{al}$ is changed very slowly, giving the buildup of input solids a chance to partially counteract the effect of the
primary air increase.

When $K_{al}$ is increased, the char bed will start to burn down. The char bed level control system compensates for this by lowering the spray temperature. Figure 23 shows a simplified flow diagram for the automatic gain adjustment program, PTIGN.

The liquor spray temperature $T_{bl}$ is being cycled in a temperature band of constant bandwidth with $T_{lhi}$ and $T_{ll0}$ as its higher and lower limits respectively. The temperature band can be moved in a region restricted below by $T_{lmin}$, where $T_{lmin}$ is slightly higher than the roping temperature $T_{lr}$.

The gain adjustment program moves the band lower limit $T_{ll0}$ towards a desired temperature $T_1$. $T_1$ is slightly higher than $T_{lmin}$, but still so low that very little entrainment of the liquor spray occurs. A diagram of the various temperature limits is shown in Figure 24 and Figure 25 where the cycling liquor temperature has been indicated.

The program in Figure 23 functions in the following way:

1. By observing the current value of $T_{ll0}$ the gain adjustment program can determine if an adjustment in the primary air gain should be made.

2. If $T_{ll0}$ is less than $T_1$, $T_{ll0}$ should be increased. The primary air gain $K_{al}$ is decreased by $\Delta K_{al}$. This will decrease the combustion rate in the char bed, and the char bed level will begin to increase. The char bed level control system will compensate by first raising the liquor temperature, and later by increasing $T_{ll0}$.

3. The program waits a time period $t_1$ to allow $T_{ll0}$ to change.
FIGURE 23
Simplified Flow Diagram
For the Automatic Gain Adjustment Program, PRIGN
FIGURE 24.
HIGH LIQUOR TEMPERATURE BAND

FIGURE 25.
DESIRED LIQUOR TEMPERATURE BAND
4. If $T_{ll0}$ has not increased the procedure is repeated from Point 2.

5. If $T_{ll0}$ has increased but is still less than $T_1$, the procedure is repeated from Point 3.

6. If $T_{ll0}$ is larger then $T_1$, then the procedure is exactly the reverse of the one just described.

The parameters $T_1$, $\Delta K_{al}$, $t_1$ and $t_2$ must be found experimentally.

AIR PORT PLUGGING DETECTION

The state of plugging of the air ports can be measured by comparing the differential pressure across the air ports to the square of the air flow through the port. The ratio of the differential pressure to the square of the flow should be independent of the flow as long as the state of clogging is unchanged. As the clogging increases, the differential pressure will increase if the flow is kept constant. Automatic cleaning may be performed either regularly at constant intervals, - or when a certain degree of restriction of the air ports is detected. The cleaning may be performed by mechanical means, or possibly by a system of steam nozzles in the air ports.

It would be impractical to have separate flow and pressure differential meters for every air port. Instead one may divide the primary and secondary windboxes into a number of regions, - one for each side of the furnace, and separately measure air flow into and pressure in each region. The furnace pressure may serve as the downstream pressure, since it is the same for all air ports.
As the windbox dampers change the orifice coefficient of air ports, compensation must be performed for variations in the damper settings.

**REPLACEMENT OF CONVENTIONAL CONTROL LOOPS WITH D.D.C.**

The several conventional control loops in the present control system are to remain functionally the same. The analog hardware may be replaced by an equivalent digital algorithm, and the control computer can then take over the task of controlling. In some cases, for the most critical control loops, it may be advisable to have analog back-up equipment. The most critical control loops are the black liquor temperature controller and the feedwater controller. The present conventional control loops encompass the precipitator and the cascade evaporator level controllers, the cascade evaporator density controller, the black liquor temperature and flow controllers, the furnace combustion air controllers, the furnace draft controller, and the feedwater and boiler level controllers. In the present control system they are all proportional - integral controllers. A digital algorithm which may be used to substitute for the analog P-I controllers is the incremental algorithm

\[
\Delta m = K_p\left[e_n - e_{n-1} + K_I \cdot e_n \cdot \Delta t\right]
\]

where \(\Delta m\) is the change in the actuator signal at time increment \(n\), and \(e_n\) and \(e_{n-1}\) are the differences between the set point signal and the measurement at time increment \(n\) and \(n-1\) respectively. \(\Delta t\) is the time increment duration, and \(K_p\) and \(K_I\) correspond to the
proportional and the integral gain respectively. Choosing a small time increment relative to the dynamics of the control loop will cause the digital controllers to act almost as the analog, and the effects of the control actions on the system will be the same.
CONTROL OF CAUSTICIZING AND SETTLING OPERATIONS

As can be seen from the discussions of Sections VII and VIII, the objective in control of the causticizing and settling operations is to attain the required white liquor and lime mud production while achieving the maximum possible settling velocity of the lime mud particles is the clarifier-thickeners. This means control of reactant addition (slaked lime and green liquor) and reaction temperature in the causticizers to achieve maximum particle sizes.

Control of the variables of these units will be carried out by standard direct digital control techniques (DDC) based on set points generated by the economic optimization or supervisory control program. No special advanced control loop algorithms are expected to be necessary for these parts of the plant.
A DESIGN OF AN OPTIMAL CONTROLLER FOR THE ROTARY LIME KILN AND RELATED UNITS

The controller for the lime kiln is designed for two typical situations: (1) to voluntarily change the operating point of the kiln to another value; and (2) to keep the values of the system variables as close as possible to the desired values specified by the operating point in the face of external upsets. The additional goals of the design are that the total amount of lime produced is maximized, while the cost due to the fuel consumed is minimized. The above requirements are used to specify the performance index for the kiln.

The mathematical model (plant equation) to be used in the design of the controllers is governed for Case (1) by Equations (12) and (13) of Section VIII and for Case (2) by the equations which result from the linearization of these same equations about an operating point. The controller for Case (1) is called a primary or servo controller and that for Case (2) a secondary or regulatory controller.

A control-input function which satisfies simultaneously the process system, i.e., the partial differential equation, Equation (12), and the algebraic equations, Equation (13) while minimizing the chosen performance measure is called an optimal control.

Due to the absence of more complete instrumentation on the kiln, the following method of attack must be used. First, an open-loop optimal control is determined for both Cases (1) and (2). An open-loop control is an explicit function of time and of the
initial and boundary conditions on the process. On the other hand, a feedback control is a function of the current state of the system and possibly of time. A controller of this latter type is designed after the optimal open-loop control has been obtained and using its results. This optimal control provides a measure of the ideal performance, which can then serve as the reference in the design of a more practical, simplified, and physically-realizable controller.

The control variables in the system representing the behavior of the kiln must be such that the choice of their values influences all state variables in the system. That is, all the quantities important to the effective operation of the kiln must be controllable either directly or indirectly by manipulation of the control variables. The following variables have been chosen as the basic controls: fuel rate, nitrogen gas rate, kiln speed and burden mass feed rate.

The determination of the optimal open-loop control is performed by solving the necessary conditions for the optimal solution of both Cases (1) and (2). The possible computational schemes for determining a candidate for the optimal control action are discussed below.

NECESSARY MATHEMATICAL CONDITIONS FOR DETERMINING AN OPTIMAL (PRIMARY) CONTROL

The partial differential equation which describes the plant can be rewritten as follows:

$$\frac{\partial q(t,t)}{\partial t} = A_0(q,u,l) \frac{\partial q(t,t)}{\partial l} + F_1(q,u,l)$$  \hspace{1cm} (60)
where \( t \in (t_0, t_f) \), a specified time interval, \( \ell \in (\ell_0, \ell_f) \), the spatial domain represented by the axial length of the kiln, and \( A_0(\cdot) \) is a \( 9 \times 9 \) diagonal matrix which has a non-vanishing determinant and is a piecewise \( C^1 \) function in \( q_1, u \), and \( \ell \), i.e., the first derivatives of the continuous function \( A_0 \) with respect to \( q \), \( u \), and \( \ell \) are defined and continuous except at a finite number of points.

The algebraic constraints are expressed in component form as follows:

\[
q_i(\ell_f, t) - g_i(t) = 0 \quad i = 4, 5, 6 \text{ and } 8 \quad (61)
\]

\[
q_i(\ell_0, t) - g_i(t) = 0 \quad i = 1, 2, 3 \text{ and } 7 \quad (62)
\]

\[
g_u(q_0(\ell_0, t), u(t)) = 0 \quad (63)
\]

\[
q(\ell, t_0) - g_0(t) = 0 \quad (64)
\]

\[
g_c(q(\ell, t)) = 0 \quad (65)
\]

where Equations (61), (62) and (63) represent boundary conditions on the distributed states; the \( g_i \)'s are piece-wise continuous functions of \( t \) and \( g_u \) is a piece-wise continuous function of \( q \) and \( u \). Equation (64) specifies the initial distributed-parameter state over the entire kiln; and \( g_0 \) is a piece-wise continuous function of \( \ell \); and function \( g_c \) is piece-wise continuous in \( \ell \).

On the basis of the desired objectives of the control action mentioned earlier the performance measure is chosen as:

\[
J(u(t)) = \frac{1}{2} \int_{t_0}^{t_f} \| u(t) \|_W^2 \, dt + \frac{1}{2} \int_{\ell_0}^{\ell_f} \| q(\ell, t_f) \|_W^2 \, d\ell
\]
where $W_u$ is pre-determined, constant, positive-definite matrix of dimension $4$, $W_q$ is a positive semi-definite pre-determined constant matrix of dimension $9$ and $W_p$ is a pre-determined constant. The first term on the right of Equation (66) represents a quadratic cost on the control variables; for example, the cost of the fuel consumed is included in this term. The second term on the right of Equation (66) is the quadratic cost of the difference between the actual states corresponding to a specific operating point at the final time, $t_f$, and the desired operating point. The operating point is here specified as a function of $t$, the spatial variable of the kiln. The last term in Equation (66) represents the dollar value of the output of the kiln, i.e., the value of the final product lime as pounds of CaO. The time interval $(t_0, t_f)$ is chosen sufficiently large, approximately equal to the unit response.

The problem is to find an optimal control function $u^*(t)$ such that $J(u)$ defined by Equation 66 is minimized, while the process system Equations ((60) to (65)) are satisfied. An outline of the derivation of $u^*(t)$ using the calculus of variations is as follows:

First, a new performance measure is defined with the constraints on interior variable values added to the original performance measure. Thus, the augmented performance measure becomes:

$$J_a(u) = \int_{t_0}^{t_f} \int_{t_0}^{t_f} \{ \lambda(t,t)^T \left[ \frac{\partial q(t,t)}{\partial t} - A_0(q,u,t) \frac{\partial q(t,t)}{\partial \lambda} \right]$$
-106-

\[-F_1(q,u,t) + \mu(t,t) g_i(q(t,t), u(t)) \right\} dt \left dt

+ \int_{t_0}^{t_f} \alpha(t) g_u(q(i_0,t), u(t)) dt

+ \frac{1}{2} \int_{t_0}^{t_f} u(t) dt + \frac{1}{2} \int_{t_0}^{t_f} q(t,t_f) - q_d(t) \right dt

- \frac{1}{2} \int_{t_0}^{t_f} W_p (u^2(t) q_2 (i_f,t)) dt \right dt

(67)

where \(\lambda(t,t), \mu(t,t)\) and \(\alpha(t)\) are multiplier functions of appropriate dimensions and the superscript \((T)\) indicates the transpose of the matrix.

Performing variations on \(\lambda(t,t), q(t,t), \mu(t,t), u(t)\) and \(\alpha(t)\) about optimal values and setting the variation of \(J^a(u^*)\) to zero, where superscript * represents an optimal value, the necessary conditions are obtained as:

\[
\frac{\partial q^*(t,t)}{\partial t} = A_0(q^*,u^*,t) \frac{\partial q^*(t,t)}{\partial t} + F_1(q^*,u^*,t)
\]

(68)

where \(t \in (t_0,t_f)\) and \(t \in (t_0,t_f)\).

\[
\frac{\partial \lambda^*(t,t)}{\partial t} = A_0^T(q^*,u^*,t) \frac{\partial \lambda^*(t,t)}{\partial t} + \frac{\partial A_0^T(q^*,u^*,t)}{\partial t} \lambda^*(t,t)
\]

\[
- A_q^T(q^*,u^*,\frac{\partial q^*}{\partial t}) \lambda^*(t,t) + \left( \frac{\partial g_u(q^*)}{\partial q} \right)^T \mu^*(t,t)
\]

(69)

where \(t \in \Gamma = (t_0,t_f) - \{t_d^j\}, j = 1,2,\) and \(t \in (t_0,t_f)\) where \(\{t_d^j\}\) represents the points in the interval \((t_0,t_f)\) at which the derivatives of \(A_0(\cdot)\) and \(F_1(\cdot)\) have discontinuities. Specifically, the
discontinuities occur at $t = t_{CA}$, the end of the chain section, and $t = t_b$ the beginning of the combustion zone.

Further,

$$- \int_{\Gamma} T(q^*, u^*, \frac{\partial q^*}{\partial t}, t) \lambda^*(l, t) \, dl + W_u u^*(t)$$

$$= \left[ W_p(q_f^*(t), t) u_z^*(t) \right] + \left( \frac{\partial q_u(q_f(t), u^*(t))}{\partial u} \right)^T \alpha^*(t) = 0$$

(70)

where the third term in Equation (70) is a $4^{th}$ order column vector.

$$g_c(q^*(t, t)) = 0$$

(71)

The boundary conditions are specified by Equation (61) through Equation (64) and also by

$$\lambda^*(l_0, t) = \left[ \frac{-1}{(A_0(q^*, u^*, t))_{99}} \right] \left[ \frac{\partial q_u(q_f(t), u^*(t))}{\partial q} \right]^T \alpha^*(t)$$

(72)

$$\lambda^*_1(l_0, t) = 0 \quad i = 4, 5, 6 \text{ and } 8$$

(73)

$$\lambda^*_1(l_0, t) = \lambda^*(l_c, t)$$

(74)

$$\lambda^*(l_b, t) = \lambda^*(l_b^+, t)$$

(75)

$$\lambda^*_2(l_f, t) = \left[ \frac{W_p(u_z^*(t))^2}{(A_0(q^*, u^*, t))_{22}} \right] q_2^*(l_f, t)$$

(76)

$$\lambda^*_1(l_0^f, t) = 0 \quad i = 1, 3, 7 \text{ and } 9$$

(77)

$$g_u(q_f^*(l_0, t), u^*(t)) = 0$$

(78)
\[ x^*(\ell, t_f) = -W_q(q^*(\ell, t_f) - q_d(\ell)) \]  

(79)

The double subscript notation indicates the row and column of the matrix \( A_0 \). The \( i^{th} - j^{th} \) elements of the matrixes \( \tilde{A}_q \) and \( \tilde{A}_u \) are defined as follows:

\[
(A_q)_{ij} = \sum_{k=1}^{9} \left[ \frac{\partial A_0}{\partial q_j} \right]_{ik} \frac{\partial q_k}{\partial t} + \frac{\partial F_i}{\partial q_j} \]  

(80)

and

\[
(A_u)_{ij} = \sum_{k=1}^{9} \left( \frac{\partial A_0}{\partial u_j} \right)_{ik} \frac{\partial q_k}{\partial t} + \frac{\partial F_i}{\partial u_j} \]  

(81)

Equations (68) and (69) form a system of 18 partial differential equations with split boundary conditions in time (Equations (64) and (79)) and in the spatial coordinate, \( \ell \) (Equations (61), (62), (63), (72), (73), (74), (75), (76), (77) and (78)). In addition, constraint Equations (65) and (70) must be fulfilled. The solution of these equations gives the ideally optimal control \( u^*(t) \).

The necessary conditions must be solved numerically, for example, on a digital computer. Various algorithms are being considered on the basis of speed, accuracy and computer memory requirements.

NECESSARY CONDITIONS FOR DETERMINING AN OPTIMAL (SECONDARY) CONTROL

To design an optimal secondary control Equations (60) through (65) are linearized about some nominal solution. Then, necessary conditions are determined for the optimal control.
To obtain the linearized equations, Equations (60) through (65) are rewritten in the component form

\[
\frac{\partial q_i(t,t)}{\partial t} = \sum_{j=1}^{9} \left[ \left( A_0(q,u,t) \right)_{ij} \frac{\partial q_j(t,t)}{\partial t} \right] + F_1^i(q,u,t), \quad i = 1,2,\ldots,9.
\]

(82)

where \((A_0(q,u,t))_{ij}\) is the element from the \(i^{th}\) row and \(j^{th}\) column of matrix \(A_0\).

The boundary conditions are also written as:

\[
q_i(t_f,t) - g_i(t) = 0 \quad i = 4,5,6 \text{ and } 8 \quad (61)
\]

\[
q_i(t_0,t) - g_i(t) = 0 \quad i = 1,2,3 \text{ and } 7 \quad (62)
\]

\[
g_u(q_0(t_0,t), u(t)) = 0 \quad (63)
\]

\[
q_i(t,t_0) - g_0^i(t) = 0 \quad i = 1,2,\ldots,9. \quad (83)
\]

\[
g_c^i(q(t,t)) = 0 \quad i = 1,2,\ldots, \quad (84)
\]

The procedure for linearization of Equations (82), (61), (62), (63), (83) and (84), omitting the arguments, results in

\[
\frac{\partial q_i}{\partial t} = \sum_{j=1}^{9} \left( A_0 \right)_{ij} \frac{\partial q_j}{\partial t} + \sum_{k=1}^{9} \left[ \left( \frac{\partial F_1}{\partial q_k} \right) + \left( \frac{\partial F_1}{\partial T} \right) \frac{\partial q_k}{\partial T} \right]
\]
where \( \tilde{q} \) and \( \tilde{u} \) represent small perturbations from the nominal solution. \( T_w \) is the temperature of the inner kiln wall.

Equation (35) can be rewritten as a vector differential equation by defining

\[
(A_q)_{ij} = - (A_0)_{ij} \quad i = 1, 2, \ldots 9. \\
(A_q)_{ik} = \sum_{j=1}^{9} \left[ \left( \frac{\partial A_0}{\partial q} \right)_{ij} \frac{\partial q_j}{\partial t} \right] + \frac{\partial F_1}{\partial u_k} \frac{\partial T_w}{\partial q_k} \\
+ \frac{\partial F_1}{\partial q_k} \quad i = 1, 2, \ldots 9. \\
+ \frac{\partial F_1}{\partial u_k} \quad k = 1, 2, \ldots 9.
\]

Then, it follows that Equation (85) becomes

\[
\frac{\partial \tilde{q}(t,t)}{\partial t} + A_k(\tilde{q}, \tilde{u}, t) \frac{\partial \tilde{q}(t,t)}{\partial t} = A_q(\tilde{q}, \tilde{u}, \frac{\partial q}{\partial t}, T_w, t) \tilde{q}(t,t)
\]
If Equation (84) is eliminated, Equations (61), (62), (63) and (83) become, respectively,

\[ q_i(t) - g_i(t) = 0 \quad i = 4, 5, 6 \text{ and } 8 \quad (90) \]

\[ q_i(t) - g_i(t) = 0 \quad i = 1, 2, 3 \text{ and } 7 \quad (91) \]

\[ g_u(q, u(t)), u(t)) = 0 \quad (92) \]

\[ q_1(t, t_0) - g_0(t) = 0 \quad i = 1, 2, \ldots, 9. \quad (93) \]

where the symbol \(^{\sim}\) over a variable represents the nominal (operating point) value of that variable and \(g_u, g_0\) and \(g_1\) in the Equations (90) to (93) which describe the boundary conditions on Equation (89) are piece-wise, \(C^1\) (continuous first derivations) in all their arguments.

A performance measure is selected on the basis of the considerations discussed previously in the introductory portion of this part:

\[
\widetilde{J}(\tilde{u}(t)) = \frac{1}{2} \int_{t_0}^{t_f} \left\| \tilde{u}(t) \right\|_2^2 dt + \frac{1}{2} \int_{t_0}^{t_f} \int_{t_0}^{t_f} \left\| \tilde{q}(\lambda, t) \right\|_q^2 \lambda d\lambda dt \\
- \frac{1}{2} \int_{t_0}^{t_f} \int_{t_0}^{t_f} \left[ (\tilde{u}_{1}(t) + \tilde{u}_{2}(t)) (\tilde{q}_{1}(\lambda, t) + \tilde{q}_{2}(\lambda, t)) \right]^2 dt
\]

(94)
where $\tilde{W}_u$ and $\tilde{W}_q$ have properties similar to $W_u$ and $W_q$, respectively, and $W_p$ is a specified constant.

If the steady-state setpoint of the overall recovery system is the true optimum, then negative cost variations in the kiln are just as undesirable as increases in cost, so the use of a quadratic cost function is reasonable.

The first term on the right hand side of Equation (94) represents a quadratic cost on the perturbations of the control from the operating point. The second term on the right of Equation (94) represents the quadratic cost of the perturbations of the kiln states from their specified values at the operating point. The last term in Equation (94) is the cost of the lime output from the kiln.

By minimizing $\tilde{J}$, the optimal control will keep the system close to the operating point specified (e.g., a steady-state condition of the kiln which produces the most lime for the dollar) and still, while correcting for minor upsets of the kiln states, will maximize the total lime produced in the interval $(t_0,t_f)$, where $t_f$ is chosen to be sufficiently large.

The problem is to find an optimal control $u^*(t)$ such that $\tilde{J}$ is minimal and still satisfy the plant (lime kiln) equations, Equation (89) through Equation (93).

Somewhat as in Section VIII, an augmented performance index $\tilde{J}_a$ is defined and weak variations are performed on the appropriate variables. The first variation on $\tilde{J}_a$ is set to zero and necessary conditions are obtained. They are concisely written in the following form:
\[ \frac{\partial \tilde{g}^*(\lambda, t)}{\partial t} + A_\lambda (\hat{q}, \hat{u}, \lambda) \frac{\partial \tilde{g}^*(\lambda, t)}{\partial \lambda} = A_q (\hat{q}, \hat{u}, \frac{\partial \hat{q}}{\partial \lambda}) \tilde{q}(\lambda, t) \]

\[ + A_u (\hat{q}, \hat{u}, \frac{\partial \hat{q}}{\partial \lambda}) \tilde{u}^*(t) \]

(95)

where \( t \in (t_0, t_f) \) and \( \lambda \in (\lambda_0, \lambda_f) \).

\[ \frac{\partial \tilde{\lambda}^*(\lambda, t)}{\partial t} + A^T_\lambda (\hat{q}, \hat{u}, \lambda) \frac{\partial \tilde{\lambda}^*(\lambda, t)}{\partial \lambda} = - A^T_q (\hat{q}, \hat{u}, \frac{\partial \hat{q}}{\partial \lambda}) \tilde{\lambda}^*(\lambda, t) \]

\[ + \tilde{w}_q \tilde{q}^*(\lambda, t) \]

\[ - \frac{\partial A^T_q (\hat{q}, \hat{u}, \frac{\partial \hat{q}}{\partial \lambda})}{\partial \lambda} \tilde{\lambda}^*(\lambda, t) \]

(96)

where \( \lambda \in \Gamma, \ t \in (t_0, t_f) \) and \( \Gamma \) is as defined previously. Also

\[ - \int_{\Gamma} A^T_u (\hat{q}, \hat{u}, \frac{\partial \hat{q}}{\partial \lambda}) \tilde{\lambda}^*(\lambda, t) \, d\lambda + \tilde{w}_u \tilde{u}^*(t) + \left( \frac{\partial \hat{q}}{\partial u} \right)^T \tilde{q}^*(t) \]

\[ - W_p \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix} \begin{bmatrix} \hat{q}_2(\lambda_f, t) + \tilde{q}_2^*(\lambda_f, t) \\ \hat{u}_3(t) + \tilde{u}_3(t) \\ 0 \end{bmatrix} = 0 \]

(97)

The boundary conditions are given by Equation (90) through (93) and also by
\[
\tilde{\lambda}_9^*(t_0, t) = \frac{1}{[A^T_\lambda(\hat{q}, \hat{u}, \lambda)]_{99}} \frac{\partial \tilde{g}_u(\tilde{q}_0^*(t_0, t), \tilde{u}^*(t))}{\partial \tilde{q}_9} \tilde{\lambda}^*(t)
\]

(98)

\[
\tilde{\lambda}_1^*(t_0, t) = 0 \quad i = 4, 5, 6 \text{ and } 8
\]

(99)

\[
\tilde{\lambda}_c^*(t_0, t) = \tilde{\lambda}_c^*(t_0^+, t)
\]

(100)

\[
\tilde{\lambda}_d^*(t_0, t) = \tilde{\lambda}_d^*(t_0^+, t)
\]

(101)

\[
\tilde{\lambda}_f^*(t_0, t) = \frac{W_c(\hat{q}_c(t) + \tilde{u}_c(t))}{[A^T_\lambda(\hat{q}, \hat{u}, \lambda)]_{22}} (\hat{q}_c(t_f, t) + \tilde{u}_c(t_f, t))
\]

(102)

\[
\tilde{\lambda}_1^*(t_f, t) = 0 \quad i = 1, 3, 7 \text{ and } 9
\]

(103)

\[
\tilde{g}_u(\tilde{q}_0^*(t_0, t), \tilde{u}^*(t)) = 0
\]

(104)

\[
\tilde{\lambda}_f^*(t, t_f) = 0
\]

(105)

The form of Equations (95) through (105) and Equations (90) through (93) is similar to the form of the equations describing necessary conditions for an optimal primary controller, except the equation coefficients are functions only of \( \lambda \), the distance along the kiln from the cold end.

The physically realizable controller is determined from a
correlation analysis of the computed solution of the optimal controller system for a large number of sets of possible kiln operating conditions. The resulting equation is similar to Equation 1 for the digester in the steady-state analysis. In this case, however, the analysis considers dynamic as well as steady-state elements of the kiln behavior.
REFERENCES CITED


SECTION III
STEADY-STATE MODEL OF THE KRAFT RECOVERY CYCLE

It was readily apparent in the initial phase of this study that the Kraft recovery process could be viewed as consisting of five separate modules, each with its own set of control and response variables. Each module consists of one or more pieces of equipment and contains internal feedback and counter-current flows. Table I lists the module name and the units within each module.

While the flow diagram presented in Figure 1 is based on the Consolidated Papers Kraft Mill in Wisconsin Rapids, Wisconsin, it must be understood that the model in its present form is not based on one particular mill because the students who worked on the project obtained their data on typical units from several different locations.

Although the model must be considered as a description of a fictitious "typical" Kraft mill, the costs, flow rates and parameters are in a reasonable range so that the model definitely computes the performance of a "typical" Kraft recovery process with a capacity equivalent to the Consolidated Papers mill.

In the following parts of this Section a control vector, denoted by $U$, will be developed. The 24 components which make up this vector are the independent variables which the optimization routine must manipulate in order to find that best operating condition which will minimize the cost of running the Kraft mill.

It must be clearly understood that a portion of the set of these
### TABLE I

**KRAFT RECOVERY MODULES**

<table>
<thead>
<tr>
<th>Module Name</th>
<th>Equipment</th>
</tr>
</thead>
<tbody>
<tr>
<td>Digester</td>
<td>Digester</td>
</tr>
<tr>
<td></td>
<td>Blow Tanks</td>
</tr>
<tr>
<td></td>
<td>Brown Stock Washer</td>
</tr>
<tr>
<td>Evaporator</td>
<td>Oxidation Tower</td>
</tr>
<tr>
<td></td>
<td>Multi-effect Evaporators</td>
</tr>
<tr>
<td>Furnace</td>
<td>Recovery Furnace</td>
</tr>
<tr>
<td></td>
<td>Cascade Evaporator</td>
</tr>
<tr>
<td></td>
<td>Electrostatic Precipitator</td>
</tr>
<tr>
<td></td>
<td>Black Liquor Heaters</td>
</tr>
<tr>
<td></td>
<td>Salt Cake Mix Tank</td>
</tr>
<tr>
<td>Green Liquor</td>
<td>Smelt Dissolving Tank</td>
</tr>
<tr>
<td>Clarification</td>
<td>Green Liquor Clarifier</td>
</tr>
<tr>
<td></td>
<td>Dregs Filter</td>
</tr>
<tr>
<td>Causticizing</td>
<td>Slaker-classifier</td>
</tr>
<tr>
<td></td>
<td>Causticizing Tanks</td>
</tr>
<tr>
<td></td>
<td>White Liquor and Lime Mud Filter</td>
</tr>
<tr>
<td></td>
<td>Rotary Lime Kiln</td>
</tr>
<tr>
<td></td>
<td>Lime Mud Thickener</td>
</tr>
</tbody>
</table>
(C) WOOD CHIPS

(C) CHEMICALS

(L) EMISSIONS

DIGESTER

STORAGE

CAUSTICIZING

CaCO₃ → CaO

FJEL(C) → KILN

W.L. → W.L.

G.L. → G.L.

WATER(C)

CLARIFICATION

EMISSIONS(L)

B.L. = BLACK LIQUOR

G.L. = GREEN LIQUOR

W.L. = WHITE LIQUOR

TERMINAL

TERMINAL

(C) = OPERATING COST

(L) = ECONOMIC LOSS

(R) = REVENUE

STEAM(C) (L)EMISSIONS STEAM(R) (L)EMISSIONS

WASHING

OXIDATION

EVAPORATION

COMBUSTION

SMELT

(F) = IMPORTANT FACTORS

FIGURE 1. KRAFT RECOVERY SYSTEM
variables which are in the control vector are not necessarily true independent control variables as defined by a process control engineer. In a sense some of these variables should be viewed as set-point variables, i.e., variables which can be monitored and directly controlled via a simple feedback system. For example, the temperature of the gas leaving the furnace is considered an independent variable by the optimization. To a control engineer the gas temperature is a set-point variable which can be maintained at a specified figure by adjusting the position of a vane which directs the furnace gases across the economizer tubes. Likewise, the temperature of the black liquor at the spray nozzles is treated as an independent variable in the model formulation; however, the true control is the amount of steam added at the black liquor heaters to raise the liquor to that temperature.

The majority of the parameters comprising the control vector are independent variables which can be manipulated directly at the mill. As discussed above, some cases exist where the parameter is really a set-point variable. Thus, the philosophy of the control vector (in the sense of the optimization) is to provide a set of variables which can be independently manipulated at the mill in order to match the performance determined by the results of the optimization, whether those variables are true control variables or variables which have set-points that can be independently maintained.

Also included in each Part of this Section is a definition of a state vector for each module which represents the component flows of the liquor in each module and may also include other
important flow rate or temperature variables: in essence, the state vectors represent the important independent variables for the kraft mill. The equations within this Section are the basic relationships necessary for computing the state vectors.
DIGESTER MODULE

The digester module cannot be easily recast into an explicit set of equations as was done with most of the other modules. However, the model for this section of the kraft mill has been simplified into a state formulation.

VARIABLE DEFINITIONS

The state vector describing the black liquor flow from the digester flash tank to the oxidation tower is given by

\[
\mathbf{X}_D = \begin{bmatrix}
\mathbf{X}_D(1) \\
\mathbf{X}_D(2) \\
\mathbf{X}_D(3) \\
\mathbf{X}_D(4) \\
\mathbf{X}_D(5) \\
\mathbf{X}_D(6) \\
\mathbf{X}_D(7)
\end{bmatrix} = \begin{bmatrix}
w_{bl}X_{blw} \\
w_{bl}X_{bls}X_{Na} \\
w_{bl}X_{bls}X_{O} \\
w_{bl}X_{bls}S \\
w_{bl}X_{bls}G \\
w_{bl}X_{bls}H \\
w_{bl}X_{bls}
\end{bmatrix} \quad (1)
\]

which represents, in order, the flow of water, sodium, oxygen, sulfur, carbon, hydrogen and solids in the black liquor leaving the flash tanks of the digester. The units are lb/hr.

The state of the white liquor flow to the digester after makeup is defined by
\[
\begin{bmatrix}
XWL(1) \\
XWL(2) \\
XWL(3) \\
XWL(4) \\
XWL(5)
\end{bmatrix} = 
\begin{bmatrix}
W_{Wl}^{(mu)}X_{N_{a2} CO_{3}}^{(mu)} \\
W_{Wl}^{(mu)}X_{N_{a2} S}^{(mu)} \\
W_{Wl}^{(mu)}X_{N_{a2} SO_{4}}^{(mu)} \\
W_{Wl}^{(mu)}X_{W}^{(mu)} \\
W_{Wl}^{(mu)}X_{NaOH}^{(mu)}
\end{bmatrix}
\]

where the units are lb/tadp.

The control vector for the digester module is

\[
U = \begin{bmatrix}
U(15) \\
U(16) \\
U(17) \\
U(18) \\
U(19) \\
U(20) \\
U(21) \\
U(22) \\
U(23) \\
U(24)
\end{bmatrix} = \begin{bmatrix}
CMRP & M & M & M & M & M & M & M & M & M
\end{bmatrix}
\]

where \(U(15)\) is the chip meter rate (rpm), \(U(16)\) is the white liquor effective alkali (lb/gal), \(U(17)\) is the white liquor sulfidity, \(U(18)\) is the lower heater temperature (°F), \(U(19)\) is the digester bypass flow (gpm), \(U(20)\) is the blow flow (gpm), \(U(21)\) is the wash temperature (°F), \(U(22)\) is the extraction flow to the flash...
tank (gpm), \( U(23) \) is the white liquor flow (gpm), and \( U(24) \) is the wash water to the brown stock washer (gpm).

There are also three parameters which are input disturbance variables to the digester. A disturbance is interpreted as a condition over which the digester operator has no control. The disturbance vector for the digester model is

\[
D = \begin{bmatrix}
D(1) \\
D(2) \\
D(3)
\end{bmatrix} = \begin{bmatrix}
\frac{W(c)X(c)}{W(mu)X(mu)} / 8.337 \\
\frac{W(c)X(c)}{W(mu)X(mu)} / 8.337 \\
\frac{W(bsw)X(bsw)}{W(bsw)X(bsw)} / 8.337
\end{bmatrix}
\] (4)

where \( D(1) \) and \( D(2) \) are the concentrations of salt cake and sodium carbonate in the white liquor (lb/gal) and \( D(3) \) is the flow of solids in the brown stock washer filtrate (lb/gal).

A general digester model can be developed using the following regression equation:

\[
Y(i) = B_0 + \sum_{j=1}^{3} B_{1j} U(j+1) + \sum_{j=4}^{6} B_{1j} D(j-3) + \sum_{j=7}^{12} B_{1j} U(j+11)
\] for \( i = 1, \ldots, 18 \) (5)

where the \( Y(i) \) are eighteen variable outputs of digester regression model.

STATE OF BLACK LIQUOR FROM FLASH TANK

The term specifying the black liquor flow to the oxidation tower can be written as follows:
Water: \( XD(1) = 500.22Y(17) \)  \( (6) \)

Sodium: \( XD(2) = 60 \cdot Y(17)(0.575Y(13)+Y(14)) \)  \( (7) \)

Oxygen: \( XD(3) = 60 \cdot Y(17)(0.4Y(13)+0.533Y(15)+0.298Y(16)) \)  \( (8) \)

Sulfur: \( XD(4) = 60 \cdot Y(17)(0.8Y(14)) \)  \( (9) \)

Carbon: \( XD(5) = 60 \cdot Y(17)(0.4Y(15)+0.644Y(16)) \)  \( (10) \)

Hydrogen: \( XD(6) = 60 \cdot Y(17)[0.025(Y(13)+Y(14)) + 0.067Y(15)+0.058Y(16)] \)  \( (11) \)

Solids: \( XD(7) = \sum_{i=2}^{6} XD(i) \)  \( (12) \)

BROWN STOCK WASHER PERFORMANCE

In order to determine (1) the amount of dissolved solids which is in the filtrate flow from the brown stock washer and (2) the sodium loss leaving with the pulp flow, a split parameter is defined for each equivalent filter bed of an idealized steady-state model of the washer. The split parameter for the first equivalent filtration is

\[
X_D^{(1)} = \frac{W_{fs}}{W_p^{(bt)}(1-X_{pf}^{(bt)})} \]

\( (13) \)

where the numerator is the flow of filtered liquor from the first filter bed and the denominator represents the total filterable flow to the washer.
The second split coefficient specifies the fraction of the filterable flow to the second filter bed which is recovered.

\[
K_b^{(2)} = \frac{W_{f2}^{(bsw)}}{W_p^{(bmt)}(1-X_{pf}^{(bmt)})}
\]  

(14)

where the numerator is the flow of filtrate from the second filter bed and the denominator is the total filterable flow to the second filter bed.

WHITE LIQUOR MAKEUP

It is common practice at some kraft mills to adjust the effective alkali and sulfidity of the white liquor to the amounts desired for good pulp production at the digester by changing the amount of salt cake addition at the cascade evaporator and by adding sodium hydroxide and/or water to the white liquor at the white liquor storage tank prior to its being pumped to the digester. Another possibility which the mills do not consider is to also add sodium sulfide at the white liquor storage tank instead of saltcake at the recovery area. The advantage of this method is the reduction of the potential load to the kiln and a possible increase in causticizing efficiency; the disadvantage is the higher cost for sodium sulfide over salt cake. Since the objective is to find the minimal cost of operation, this option has been included. Thus, the makeup section of the model adjusts the effective alkali, sulfidity and volumetric flow of the white liquor to the amounts specified by U(15), U(17), and U(23) during the optimization. Any
excess white liquor is considered revenue, i.e., it is good liquor which could be stored and used when an increased flow rate of white liquor is required.

If the white liquor flow is less than the specified amount, then the amount of water addition is

$$w_w^{(\text{mul})} = U(23) - XWLC(4)$$ (15)

where $XWLC(4)$ has been converted to units of gpm. If the white liquor flow exceeds the specified amount, then the fractional excess of white liquor is

$$X_{w_l}^{(\text{ex})} = 1 - \frac{U(23)}{XWLC(4)}$$ (16)

and the amount of excess white liquor is

$$EXWL(i) = X_{w_l}^{(\text{ex})} \cdot XWLC(i) \quad i = 1, \ldots, 5$$ (17)

where $EXWL$ is a (5x1) vector containing the excess amounts of sodium carbonate, sodium sulfide, sodium sulfate, water and sodium hydroxide respectively. If there is no excess, then the elements of this vector are zero.

If the sulfidity is too low, then the amount of sodium sulfide as equivalent sodium in sodium hydroxide is

$$\frac{1.026[XWLC(2) + W^{(\text{mul})}_{\text{Na}_2S}]}{1.026[XWLC(2) + W^{(\text{mul})}_{\text{Na}_2S} + XWLC(5)]} = U(17)$$ (18)
where $W_{Na_2S}^{(mul)}$ is the required amount of sodium sulfide necessary to adjust the sulfidity of the white liquor to the value specified by $U(17)$ and the constant 1.026 is the conversion factor for sodium sulfide to sodium hydroxide in equivalent sodium. Solving for sodium sulfide addition

$$W_{Na_2S}^{(mul)} = \frac{U(17)}{1.026[1-U(17)]} \times WLC(5) - WLC(2)$$

where the units of $W_{Na_2S}^{(mul)}$ are lb/tadp.

If the sulfidity is too high, it can be decreased by adding sodium hydroxide. Thus,

$$\frac{1.026 \times WLC(2)}{1.026 \times WLC(2) + WLC(5) + W_{NaOH}^{(mul)}} = U(17)$$

and

$$W_{NaOH}^{(mul)} = 1.026 \times WLC(2) \left[ \frac{1}{U(17)} - 1 \right] - WLC(5)$$

If the effective alkali is too low, then sodium hydroxide and sodium sulfide must be added in the ratio specified by the sulfidity control variable. Thus,

$$W_{NaOH}^{(mu2)} = [1-U(17)] [U(16)-WLEA]$$

and

$$W_{Na_2S}^{(mu2)} = 0.513 \ U(17) [U(16)-WLEA]$$
where \( W_{LEA} \) is the white liquor effective alkali (lb/gal) after adjustment for sulfidity, \( U(16) \) is the specified effective alkali and the variables \( W_{NaOH}(\mu_2) \) and \( W_{Na_2S}(\mu_2) \) are the additional sodium hydroxide and sodium sulfide which must be added above that specified by Equations 17 and 18.

If the effective alkali is too high, then water must be added.

\[
W_{W}(\mu_2) = \left\{ \frac{W_{LEA}}{U(16)} - 1 \right\} U(23)
\]

where \( W_{W}(\mu_2) \) represents the required water addition above that specified by Equation 15. Also, since the volumetric flow of the white liquor now exceeds that specified by \( U(23) \), it must be readjusted via Equations 16 and 17.

Thus the state of the white liquor to the digester is

\[
\begin{align*}
\text{Na}_2\text{CO:} & \quad XWL(1) = XWLC(1) - EXWL(1) \\
\text{Na}_2\text{S:} & \quad XWL(2) = XWLC(2) + W_{Na_2S}(\mu_1) + W_{Na_2S}(\mu_2) - EXWL(2) \\
\text{Na}_2\text{SO}_4: & \quad XWL(3) = XWLC(3) - EXWL(3) \\
\text{Water:} & \quad XWL(4) = XWLC(4) + W_{W}(\mu_1) + W_{W}(\mu_2) - EXWL(4) \\
\text{NaOH:} & \quad XWL(5) = XWLC(5) + W_{NaOH}(\mu_1) + W_{NaOH}(\mu_2) - EXWL(5)
\end{align*}
\]

**DISTURBANCE VARIABLES**

The amount of salt cake as sodium hydroxide in equivalent sodium per gallon of water in the white liquor is

\[
D(1) = 0.563 XWL(3)/(XWL(4)/8.337)
\]
and the amount of sodium carbonate as sodium hydroxide in equivalent sodium per gallon of white liquor is

$$D(2) = 0.755W_L(1)/(XWL(4)/8.337)$$  \hspace{1cm} (31)

To determine the amounts of solids per gallon of filtrate from the brown stock washer,

$$w_{bl1}(bsw)x_{blsw} = k_b(1)+k_b(2)(1-k_b(1)) w_{p1}(bt)x_{ps}$$  \hspace{1cm} (32)

$$w_{bl1}(bsw)x_{blsw} = [k_b(1)+k_b(2)(1-k_b(1))] w_{p1}(bt)x_{w}$$  \hspace{1cm} (33)

The solids concentration in the filtrate in lb/gal is

$$D(3) = w_{bl1}(bsw)x_{blsw}/w_{bl1}(bsw)x_{blsw}/8.337$$  \hspace{1cm} (34)

**SODIUM LOSS AT THE BROWN STOCK WASHER**

The sodium loss at the washer does not appear in the performance index since it cannot be considered a pollutant to the ambient surroundings and the cost of chemical addition for makeup is considered at another point. It is still an important parameter, however, since it is, in effect, a measure of the washing efficiency. Further, the sodium carried with the pulp constitutes a cost to the bleach plant since more chemicals are required than the case of sodium-free pulp flow. The sodium loss is

$$w_{bl1}(bsw)x_{ps}x_{Na} = 1 - [k_b(1)+k_b(2)(1-k_b(1))] w_{p1}(bt)x_{ps}x_{Na}$$  \hspace{1cm} (35)
SOLUTION PROCEDURE

The technique used to determine the outputs of the digester module was to treat the model as a physical flow problem.
EVAPORATOR MODULE

Since the only change in black liquor content is due to the evaporation of water, the model for the oxidation tower and multiple effect evaporators is a set of equations representing the transfer of black liquor from the digester to the output side of the evaporators with water being the only variable which changes in value. Since the Consolidated Papers kraft mill, on which the model is generally based, produces only negligible amounts, soap production is not considered in this particular formulation. It could be added.

VARIABLE DEFINITIONS FOR THE EVAPORATOR MODULE

The state vector for the liquor leaving the multiple effect evaporators is defined as

\[
X_E = \begin{bmatrix}
X_E(1) \\
X_E(2) \\
X_E(3) \\
X_E(4) \\
X_E(5) \\
X_E(6) \\
X_E(7)
\end{bmatrix} = \begin{bmatrix}
W_{bl}x_{blw} \\
W_{bl}x_{bls}x_{Na} \\
W_{bl}x_{bls}x_{O} \\
W_{bl}x_{bls}x_{S} \\
W_{bl}x_{bls}x_{C} \\
W_{bl}x_{bls}H \\
W_{bl}x_{bls}
\end{bmatrix}
\]

where the states represent, in order, the flow of water, sodium, oxygen, sulfur, carbon, hydrogen and solids in the black liquor.
The notation in the right-most column vector is defined at the end of this Section. The units are lb/hr.

The solids flow is comprised of the sum of the elemental flows in the black liquor. Thus, an auxiliary relationship is

\[ XE(7) = \sum_{i=2}^{6} XE(i) \]  (37)

The control vector for the evaporator module is

\[ U = \begin{bmatrix} U(1) \\ U(2) \end{bmatrix} = \begin{bmatrix} \eta_{ot} \\ W_{s}^{(1)} \end{bmatrix} \]  (38)

where \( U(1) \) is the oxidation efficiency of the oxidation tower and \( U(2) \) is the plant steam supplied to the first effect of the evaporators (lb/hr). Since the control variables will be the manipulated parameters in the optimization, they will be numbered sequentially through the modules in order to correspond with the notation in the computer programs.

Although the oxidation efficiency is not an actual control variable, it was felt that a "handle" should be provided to include the performance of the oxidation tower. Hopefully, a more accurate model relating oxidation efficiency to the true independent variables of the tower can be incorporated when the operation of this unit is better understood.
MATHEMATICAL MODEL FOR EVAPORATOR MODULE

Once the steam economy of the evaporators has been determined by separate computations, the total amount of water evaporated from the liquor can be computed using the relation

\[ W_e = SE \cdot U(2) \]  
\hspace{1cm} (39)

where SE represents the steam economy for the system.

The set of equations describing the liquor flow from the digester through the evaporator module are

Water: \[ XE(1) = XD(1) - W_e \]  
\hspace{1cm} (40)

Sodium: \[ XE(2) = XD(2) \]  
\hspace{1cm} (41)

Oxygen: \[ XE(3) = XD(3) \]  
\hspace{1cm} (42)

Sulfur: \[ XE(4) = XD(4) \]  
\hspace{1cm} (43)

Carbon: \[ XE(5) = XD(5) \]  
\hspace{1cm} (44)

Hydrogen: \[ XE(6) = XD(6) \]  
\hspace{1cm} (45)

Solids: \[ XE(7) = XD(7) \]  
\hspace{1cm} (46)

where the first term in the right side of Equation 40 and the right side of Equations 41-46 represent the corresponding flow from the digester (lb/hr).

The amount of gaseous emissions from the evaporators rewritten in terms of the oxidation efficiency as a control variable are

\[ W_{SO_2}^{(ev)} = 0.0625 \cdot U(1) + 0.005 \]  
\hspace{1cm} (47)

\[ W_{H_2S}^{(ev)} = -1.794 \cdot U(1) + 1.55 \]  
\hspace{1cm} (48)
\( \text{CH}_2\text{SH}: \quad w_{\text{RSH}}^{(\text{ev})} = -0.75 \ U(1)+0.8 \)  

\( \text{CH}_3\text{SCH}_3: \quad w_{\text{RSSR}}^{(\text{ev})} = 0.0438 \ U(1)+0.065 \)  

\( \text{CH}_3\text{S} \cdot \text{SCH}_3: \quad w_{\text{RSSR}}^{(\text{ev})} = 0.106 \ U(1)+0.015 \)

The units are lb/ton air dry pulp (tadp). Because the amount of carbon, hydrogen, oxygen and sulfur loss due to gaseous emissions is so small relative to their amounts in the liquor, these terms are not included in the material balances.
FURNACE MODULE

Although the number of equations initially required to describe the furnace-cascade evaporator-precipitator system is quite large, numerous algebraic substitutions resulted in a reduced set of 13 basic equations plus several auxiliary relationships.

VARIABLE DEFINITIONS FOR THE FURNACE MODULE

The state vector for the furnace module is defined as

\[
\mathbf{X}_F = \begin{bmatrix}
\mathbf{X}_F(1) \\
\mathbf{X}_F(2) \\
\mathbf{X}_F(3) \\
\mathbf{X}_F(4) \\
\mathbf{X}_F(5) \\
\mathbf{X}_F(6) \\
\mathbf{X}_F(7) \\
\mathbf{X}_F(8) \\
\mathbf{X}_F(9) \\
\mathbf{X}_F(10) \\
\mathbf{X}_F(11) \\
\mathbf{X}_F(12) \\
\mathbf{X}_F(13)
\end{bmatrix} = \begin{bmatrix}
w_{bl1}(ce)X_{blw} \\
w_{bl1}(ce)X_{bls}Na \\
w_{bl1}(ce)X_{bls}O \\
w_{bl1}(ce)X_{bls}S \\
w_{bl1}(ce)X_{bls}C \\
t_{bl1} \\
w_{g}(g2)X_{H2S} \\
w_{g}(g2)X_{SO2} \\
w_{g}(g2)X_{CO} \\
w_{g}(g2)X_{CO2} \\
w_{g}(g2)X_{Na2CO3} \\
w_{g}(g2)X_{Na2SO4} \\
t_{g}(ce)
\end{bmatrix}
\] (52)
where $\mathbf{X}(1), \ldots, \mathbf{X}(6)$ is the state of the black liquor leaving the cascade evaporator (lb/hr and °F), $\mathbf{X}(7), \ldots, \mathbf{X}(12)$ is the state of the gas leaving the secondary zone of the furnace (lb/hr), and $\mathbf{X}(13)$ is the temperature of the gas leaving the cascade evaporator (°F).

The control vector for the furnace module is

$$
\mathbf{U} = 
\begin{bmatrix}
U(3) \\
U(4) \\
U(5) \\
U(6) \\
U(7)
\end{bmatrix} = 
\begin{bmatrix}
W_{sc}(ce) \\
T_{bl}(sp) \\
W_{a}(1) \\
W_{a}(2) \\
T_{g}(5)
\end{bmatrix}
$$

where $U(3)$ is the salt cake addition at the cascade (lb/hr), $U(4)$ is the temperature of the black liquor at the spray nozzles (°F), $U(5)$ and $U(6)$ are the primary and secondary air flows to the furnace (lb/hr), and $U(7)$ is the temperature of the flue gas leaving the economizer section of the boiler system in the furnace (°F).

An output vector for the furnace module can be defined as the component flow of the smelt and the steam production.

$$
\mathbf{Y}_F = 
\begin{bmatrix}
Y_F(1) \\
Y_F(2) \\
Y_F(3) \\
Y_F(4)
\end{bmatrix} = 
\begin{bmatrix}
W_{sm}X_{sm}^{(sm)}_{Na_2CO_3} \\
W_{sm}X_{sm}^{(sm)}_{Na_2S} \\
W_{sm}X_{sm}^{(sm)}_{Na_2SO_4} \\
W_{st}^{(f)}
\end{bmatrix}
$$
STATE OF THE BLACK LIQUOR LEAVING THE CASCADE

The amount of water in the black liquor leaving the cascade evaporator is defined by

\[ \text{XF}(1) = \text{XE}(1) - \text{RH}20 - 0.529 \cdot \text{RH}2S \] (55)

where \( \text{XE}(1) \) was previously defined as the amount of water in the liquor leaving the multiple effect evaporators, \( \text{RH}20 \) is the evaporation of water which takes place, and the last term is the additional amount of water lost due to the formation of hydrogen sulfide.

The water evaporation rate is defined as

\[ \text{RH}20 = \text{AKH}20 \left[ \text{XF}(13) - \text{TWH} \right] \] (56)

where \( \text{AKH}20 \) is an overall evaporation constant defined as

\[ \text{AKH}20 = \text{A}_{wh} (ce) K_{c}^{(ce)} = 294.7 \] (57)

and \( \text{TWH} \) is the temperature of the surface of the wheel and is assumed to be 236°F.

The rate expression for hydrogen sulfide generation is

\[
\text{RH}2S = \frac{\left[ \text{AKH}2S \cdot \text{PNA}2S \cdot \text{XE}(2) \right] \cdot \text{XF}(10)}{\left[ \text{XF}(1) + \text{WBLS} \right] \cdot \text{WG}5T}
\] (58)

where \( \text{AKH}2S \) is a rate coefficient, \( \text{PNA}2S \) is the lb. \( \text{Na}_2\text{S} \)/lb. \( \text{Na} \) in the liquor leaving the cascade, \( \text{XE}(2) \) is the sodium in the liquor leaving the multiple effect evaporators, \( \text{WBLS} \) is the total
solids flow in the liquor leaving the cascade and WG5T is the total gas flow from the economizer of the furnace.

Note that water addition due to diluting black liquor has not been included in Equation 55. It is assumed that dilution with weak or strong black liquor at the cascade evaporator will not be necessary.

The sodium flow in the liquor leaving the cascade is

$$XF(2) = XE(2) + 0.434 \left[ 1 - (1 - K_{pe})PFC \right] XF(11)$$
$$+ 0.324 \left[ (1 - (1 - K_{pe})XF(12) + U(13) \right] \tag{59}$$

where the constant 0.434 is twice the ratio of the atomic weight of sodium to sodium carbonate and 0.324 is twice the ratio of the atomic weight of sodium to saltcake. $K_{pe}$ is the efficiency of the precipitator and is defined by Galtung. The terms, PFC and PFS define the ratio of fumes to total flow of sodium carbonate and salt cake in the furnace gases, and are defined by Equations 86-91.

The flow of oxygen, sulfur and carbon in the liquor leaving the cascade evaporator are

$$XF(3) = XE(13) + 1.412 \cdot RH2S + 0.453 \left[ 1 - (1 - K_{pe})PFC \right] XF(11)$$
$$+ 0.452 \left[ (1 - (1 - K_{pe})PFS)XF(12) + U(3) \right] \tag{60}$$

where the second term on the right side represents the oxygen addition due to the formation of hydrogen sulfide, the constant 0.453 is three times the ratio of the atomic weight of oxygen to sodium carbonate and 0.452 is four times the ratio of the atomic weights of oxygen to salt cake.
Sulfur: \[\text{XF}(4) = \text{XE}(4) - 0.941 \cdot \text{RH}_2\text{S} + 0.225[(1-(1-K_{pe})\text{PFS})\text{XF}(12) + \text{U}(3)] \] (61)

where the constant 0.225 is the ratio of the atomic weight of sulfur to saltcake and the second term on the right side represents the sulfur loss due to the formation of hydrogen sulfide.

Carbon: \[\text{XF}(5) = \text{XE}(5) + 0.353 \cdot \text{RH}_2\text{S} + 0.113[1-(1-K_{pe})\text{PFC}]\text{XF}(11) \] (62)

where the coefficient 0.113 is the ratio of the atomic weight of carbon to sodium carbonate and the second term on the right side represents the addition of carbon due to the formation of hydrogen sulfide.

The temperature of the liquor leaving the cascade can be found by solving for \(\text{XF}(6)\) in the energy balance for the cascade liquor. Using the state formulation, let

\[Z_6 = [\text{XE}(1)+\text{XE}(7)+K_{pe}(\text{PFC} \cdot \text{XF}(11)+\text{PFS} \cdot \text{XF}(12))]c_{\text{pr}} T_{\text{pr}} \]

\[+U(3)c_{p_{sc}} T_{sc} +[(1-\text{PFC})\text{XF}(11)+(1-\text{PFS})\text{XF}(12)]c_{p_{co}} \text{XF}(13) \]

\[+UAV \cdot \text{XF}(13) + UAWH(\text{XF}(13) - \text{TWH}) \]

\[-\text{RH}_2\text{O}(H_{(\text{ce}+c_{p_w})} \cdot \text{TWH}) \]

\[V_6 = [\text{XF}(1)+\text{WBLS}]c_{p_{bl}} +UAV \] (64)

then

\[\text{XF}(6) = \frac{Z_6}{V_6} \] (65)
where the $c_p$'s are specific heats for their respective terms. The superscript ($\ell$) stands for liquid water and ($v$) for vapor.

The following table of values (Table II) for the various specific heats and heat transfer coefficients was taken from the work of Galtung (12).

STATE OF FLUE GAS LEAVING SECONDARY ZONE OF FURNACE

The generation of hydrogen sulfide and sulfur dioxide in the secondary zone of the furnace can be derived as

$$\begin{align*}
\text{H}_2\text{S:} & \quad {X}_F(7) = K_7 \cdot \eta_e \cdot {X}_F(4) \cdot \exp[-\alpha_7 \delta - \beta_7 {x}_{O_2}^{(dg^2)}] \\
\text{SO}_2: & \quad {X}_F(8) = K_8 \cdot \eta_e \cdot {X}_F(4) \cdot \exp[-\alpha_8 \delta - \beta_8 {x}_{O_2}^{(dg^2)}]
\end{align*}$$

(66) (67)

where $K$, $\alpha$, and $\beta$ are constants, $\eta_e$ is the entrainment factor, $\delta$ is a turbulence parameter, and ${x}_{O_2}^{(dg^2)}$ is the excess oxygen concentration term.

The formation of carbon monoxide in the secondary zone is

$$\begin{align*}
\text{CO:} & \quad {X}_F(9) = K_9 [ {X}_F(5) - 0.113 {Y}_F(1) ] \exp[-\alpha_9 \delta - \beta_9 {x}_{O_2}^{(dg^2)}]
\end{align*}$$

(68)

The constant 0.113 represents the ratio of the atomic weight of carbon to sodium carbonate.

The values for the three parameters in each of the above three equations were computed by Galtung (12) and are given in Table III.

The amount of carbon dioxide is

$$\begin{align*}
\text{CO}_2: & \quad {X}_F(10) = 3.667 [ {X}_F(5) - 0.113 {Y}_F(1) - 0.428 {X}_F(9) - 0.113 {X}_F(11) ]
\end{align*}$$

(69)
### TABLE II

**SPECIFIC HEAT AND HEAT TRANSFER COEFFICIENT VALUES**

<table>
<thead>
<tr>
<th>Specific Heat</th>
<th>(Btu/lb-hr-°F)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$c_{p_{co}}$</td>
<td>0.23</td>
</tr>
<tr>
<td>$c_{p_{g}}^{(5)}$</td>
<td>0.24</td>
</tr>
<tr>
<td>$c_{p_{sc}}$</td>
<td>0.23</td>
</tr>
<tr>
<td>$c_{p_{w}}^{(l)}$</td>
<td>1.0</td>
</tr>
<tr>
<td>$c_{p_{w}}^{(v)}$</td>
<td>0.48</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Heat Transfer</th>
<th>(Btu/°F)</th>
</tr>
</thead>
<tbody>
<tr>
<td>UAV</td>
<td>$1.01 \cdot 10^4$</td>
</tr>
<tr>
<td>UAWH</td>
<td>$2.9339 \cdot 10^5$</td>
</tr>
<tr>
<td>i</td>
<td>$K_i$</td>
</tr>
<tr>
<td>----</td>
<td>------------</td>
</tr>
<tr>
<td>7</td>
<td>1.121 $\cdot 10^4$</td>
</tr>
<tr>
<td>8</td>
<td>2.039 $\cdot 10^6$</td>
</tr>
<tr>
<td>9</td>
<td>6.585</td>
</tr>
</tbody>
</table>
The coefficients inside the brackets are the ratios of the atomic weights of carbon to the compound represented by the variable name. The constant 3.667 is the ratio of the molecular weight of carbon dioxide to carbon.

The total amount of sodium carbonate in the gas leaving the secondary zone of the furnace is

$$\text{Na}_2\text{CO}_3: \quad XF(11) = 2.304[\eta_e \cdot XF(2) - 0.324XF(12)] \quad (70)$$

The constant 2.304 is half the ratio of the molecular weight of sodium carbonate to sodium and the coefficient 0.324 is twice the ratio of sodium to salt cake.

The relationship for the total flow of salt cake in the gas leaving the secondary zone is

$$\text{Na}_2\text{SO}_4: \quad XF(12) = 4.444[\eta_e \cdot XF(4) - 0.941XF(7) - 0.5XF(8)] \quad (71)$$

The constant 0.941 is the ratio of the atomic weight of sulfur to hydrogen sulfide, the coefficient 0.5 is the ratio of the atomic weight of sulfur to sulfur dioxide and the constant 4.444 is the ratio of the molecular weight of salt cake to sulfur.

TEMPERATURE OF GAS LEAVING CASCADE EVAPORATOR

The temperature of the gas leaving the cascade evaporator can be computed by solving the energy balance for XF(13) in the cascade gas flow.

Let

$$T_l = XF(1)+8 \cdot XE(6) + W^{(h)}_{st} - 0.529 \cdot XF(7)$$

$$+ 0.0133 \left[ U(5) + U(6) + W^{(1)}_{ia} + W^{(2)}_{ia} \right] \quad (72)$$
\[ T_2 = (1-PFC) \cdot XF(11) + (1-PFS) \cdot XF(12) \] (73)

\[ z_{13} = \left[ (W \text{G}_5T-T_1-T_2) \cdot c_p(5) + T_1 \cdot c_p(\nu) + T_2 \cdot c_p(\nu) \right] u(5) \]
\[ + (R H_{20} \cdot c_p(\nu) + U A W H) T_{wh} + U A V \cdot XF(6) \] (74)

\[ v_{13} = (W \text{G}_5T-T_1-T_2) \cdot c_p(5) + T_1 \cdot c_p(\nu) + T_2 \cdot c_p(\nu) \] (75)

then

\[ XF(13) = z_{13}/v_{13} \] (76)

where \( w_{st}^{(h)} \) is the steam added to the liquor at the black liquor heaters, \( W_{la}^{(1)} \) and \( W_{la}^{(2)} \) are the amounts of infiltration air leaking into the primary and secondary zones, and \( W \text{G}_5T \) is the total flow of gases leaving the furnace. The superscript \( (\nu) \) stands for water vapor.

**SMELT PRODUCTION**

The smelt flow from the furnace is assumed to be made up of sodium carbonate, sodium sulfide and salt cake.

\[ \text{Na}_2\text{CO}_3: \quad YF(1) = 2.304[(1-\eta_e) \cdot XF(2) - 0.59 \cdot YF(2) - 0.324 \cdot YF(3)] \] (77)

where the coefficient 0.59 is twice the ratio of the atomic weight of sodium to sodium sulfide, the constant 0.324 is twice the ratio of the atomic weight of sodium to salt cake, and the coefficient 2.304 is half the ratio of the molecular weight of sodium carbonate to sodium. \( \eta_e \) is the entrainment coefficient.
Na₂S: \( Y_F(2) = 2.439(1-\eta_g)\eta_r \cdot X_F(4) \) (78)

where 2.439 is the ratio of the molecular weight of sodium sulfide to sodium and \( \eta_r \) is the reduction efficiency.

\( \text{Na}_2\text{SO}_4: \ Y_F(3) = 4.444(1-\eta_g)(1-\eta_r)X_F(4) \) (79)

where the constant 4.444 is the ratio of the molecular weight of salt cake to sodium.

AUXILIARY RELATIONSHIPS FOR THE FURNACE MODULE

A number of parameters have been defined in the preceding text without use of equations. In order to make the computer programs for the furnace module easier to understand, the more important parameters are defined below.

The flow of solids in the liquor leaving the cascade is given by

\[ W_{BLS} = \sum_{i=2}^{5} X_F(1) + X_E(6) \]  

(80)

The total flow of flue gas leaving the economizer of the furnace is

\[ W_{G5T} = X_F(1) + W_{BLS} + U(5) + U(6) + W_{1a}^{(1)} + W_{1a}^{(2)} + \\
W_{st} - Y_F(1) - Y_F(2) - Y_F(3) \]  

(81)

The turbulence factor for the generation Equations 66-68 is

\[ \delta = \frac{1}{\rho_a^{(2)}} \begin{bmatrix} U(6) \\ A_{po}^{(2)} \end{bmatrix} \]  

(82)
where $A^{(2)}_{po}$ is the total cross-sectional area of the secondary ports and $\rho^{(2)}_{a}$ is the density of the secondary air. The oxygen factor is defined as

$$x_{O_2}^{(dg2)} = \frac{A_2}{w^{(2)}_{gd}}$$

(83)

where $A_2$ is the oxygen excess in the secondary zone, and $w^{(2)}_{gd}$, the total flow of dry gas leaving the secondary zone, is

$$w^{(2)}_{gd} = w^{(h)}_t - 0.0133[u^{(1)} + w^{(1)}_{ia} + w^{(2)}_{ia}]$$

(84)

In Equation 84 it is assumed that 1.33% of the total air to the furnace is in the form of water vapor.

The amount of steam added at the black liquor heaters to raise the liquor temperature is given by

$$w^{(h)}_t = \frac{[x^{(1)} + WBLS] \left[ c^{(sp)}_{pbl} u^{(4)} - c^{(ce)}_{pbl} x^{(6)} \right]}{H^{(h)}_{w} + c_{pw}^{(4)} T^{(h)}_{w} - c_{pbl}^{(sp)} u^{(2)}}$$

(85)

where $H^{(h)}_{w}$ is the heat of condensation of the steam and the second term in the denominator is the sensible heat of the steam.

The following set of equations define the ratio of salt cake and sodium carbonate as fumes or particulates to the total flow of salt cake and sodium carbonate in the furnace gas.

If

$$\eta x^{(4)} - 0.941 x^{(7)} - 0.5 x^{(8)} > 0.696 d^2 x^{(2)}$$

(86)
then
\[
PFS = 3.087 \cdot d_2 \frac{XF(2)}{XF(12)}
\]  \hspace{1cm} (87)

PFC = 0.0 \hspace{1cm} (88)

If
\[
\eta_e \cdot XF(4) - 0.941 \cdot XF(7) - 0.5 \cdot XF(8) \leq 0.696 \cdot d_2 \cdot XF(2)
\]  \hspace{1cm} (89)

then
\[
PFS = 1.0
\]  \hspace{1cm} (90)

\[
PFC = \frac{2.304[d_2 \cdot XF(2) - 0.324 \cdot XF(12)]}{XF(11)}
\]  \hspace{1cm} (91)

STEAM PRODUCTION

The energy equations for the furnace, in terms of the state notation, are as follows.

Sensible heat in black liquor spray:
\[
Q_{bl} = \left[ XF(1) + WBLS + W_{st}^{(h)} \right] c_{p_{bl}} U(2)
\]  \hspace{1cm} (92)

Sensible heat in air to furnace:
\[
Q_a = \left[ U(5) + U(6) \cdot W_{la}^{(1)} + W_{la}^{(2)} \right] c_{p_a} T_a
\]  \hspace{1cm} (93)

The primary and secondary air are assumed to be at the same temperature.
Heat of combustion in primary zone:

\[ Q_c^{(1)} = \left[ \frac{W_{bls} - (1 - PFC + K_{pe} \cdot PFC) \cdot X(1) - (1 - PFS + K_{pe} \cdot PFS) \cdot X(12)}{1 - PNA2S \cdot X(4)} \right] H_{bls} \cdot \eta_r \cdot X(4) \cdot H_s - 8 \cdot \eta_e \cdot X(6) H_w \] (94)

where \( H_{bls} \) is the heat of formation of black liquor solids and \( H_w \) is the heat of formation of water. The three flows subtracted from \( W_{bls} \) represent sodium carbonate, sodium sulfide, and salt cake which do not burn.

Heat of combustion in the secondary zone:

\[ Q_c^{(2)} = Q_c^{(1)} \left[ \frac{W_{st}^{(1)}}{W_{st}^{(1)} + W_0 \cdot \eta_e \cdot W_{bls}} \right] + \eta_e \cdot W_{bls} \] (95)

where \( H_{H_2S} \) and \( H_{CO} \) are the heats of formation of hydrogen sulfide and carbon monoxide. The total energy input to the furnace is given by

\[ Q_{in} = Q_{bl} + Q_a + Q_c^{(1)} + Q_c^{(2)} \] (96)

The terms representing the energy leaving the system are

Heat of vaporization in primary zone:

\[ Q_v^{(1)} = \left[ X(1) + W_{st}^{(h)} \right] (1 - \eta_e) H_w^{(1)} \] (97)
Heat of fusion of smelt:

\[ Q_{sm}^{(f)} = [YF(1)+YF(2)+YF(3)]H_{sm} \]  \hspace{1cm} (98)

Sensible heat of smelt:

\[ Q_{sm}^{(s)} = [YF(1)+YF(2)+YF(3)]c_{p_{sm}}T_{sm} \]  \hspace{1cm} (99)

where the specific heat of smelt is 0.23 and the temperature is assumed to be 1550°F.

Heat of reduction of salt cake:

\[ Q_{sc} = (1-PFS+K_{pe} \cdot PFS) \cdot \eta_r \cdot XF(12) \cdot H_{s} \cdot (1-\eta_e) \]  \hspace{1cm} (100)

Heat of vaporization in secondary zone:

\[ Q_{v}^{(2)} = [XF(1)+W_{st}^{(h)}] \eta_e H_{w}^{(2)} \]  \hspace{1cm} (101)

Sensible heat of gas leaving the economizer:

\[ Q_{g}^{(5)} = W_{g} T_{c5} \cdot U_{g}^{(5)} \]  \hspace{1cm} (102)

The total energy loss from the furnace is

\[ Q_{out} = Q_{v}^{(1)} + Q_{sm}^{(f)} + Q_{sm}^{(s)} + Q_{sc} + Q_{v}^{(2)} + Q_{g}^{(5)} \]  \hspace{1cm} (103)

The amount of available energy for steam production is

\[ Q_{ast} = Q_{in} - Q_{out} \]  \hspace{1cm} (104)

The steam production is

\[ YF(4) = \eta_{st}^{(f)} \cdot Q_{ast} \]  \hspace{1cm} (105)
\( \eta_{st}^{(f)} \) is an efficiency factor and represents the fraction of available energy which is actually used in the production of steam.
GREEN LIQUOR CLARIFICATION MODULE

The green liquor clarification (GLC) module can be described by a set of 4 equations.

The state vector for the GLC module is defined as

\[ \mathbf{X}_G = \begin{bmatrix} \mathbf{x}_G(1) \\ \mathbf{x}_G(2) \\ \mathbf{x}_G(3) \\ \mathbf{x}_G(4) \end{bmatrix} = \begin{bmatrix} \mathbf{w}(\text{sdt})_\mathbf{x}(\text{sdt})_{\text{Na}_2\text{CO}_3} \\ \mathbf{w}(\text{sdt})_\mathbf{x}(\text{sdt})_{\text{Na}_2\text{S}} \\ \mathbf{w}(\text{sdt})_\mathbf{x}(\text{sdt})_{\text{Na}_2\text{SO}_4} \\ \mathbf{w}(\text{sdt})_\mathbf{x}(\text{sdt})_w \end{bmatrix} \] (106)

which represents the four components which make up the green liquor flowing from the smelt dissolving tank. The dregs in the green liquor are not included since the dregs flow is assumed to be an average value based on the rate of pulp production. The units are lb/tadp.

The control vector for the GLC module is

\[ \mathbf{U} = \begin{bmatrix} \mathbf{u}(8) \\ \mathbf{u}(9) \end{bmatrix} = \begin{bmatrix} \mathbf{w}(\text{sdt})_{\text{st}} \\ \mathbf{w}(\text{d})_w \end{bmatrix} \] (107)

which is the steam and condensate added at the smelt tank and the dilution and wash water supplied to the dregs filter (lb/tadp).

The factor \( \eta_{\text{GLC}} \) represents the fraction of the green liquor which passes through the clarifier and continues on to the causticizing plant.
MATHEMATICAL MODEL FOR THE GLC MODULE

The parameter $K_f$ can be considered a split coefficient defined as

$$K_f = \frac{W_{df}}{W_{df} - W_{dregs}}$$

where the numerator is the flow of filtered liquor back to the smelt tank and the denominator is the total flow of the filterable portion of the slurry to the dregs filter. It is assumed that the dregs are completely removed on the dregs filter.

$$W_{df} = (1 - \eta_{glc}) \sum_{i=1}^{4} XG(1) + U(9) + W_{dregs}$$

so that

$$K_f = \frac{W_{df}}{(1 - \eta_{glc}) \left[ \sum_{i=1}^{4} XG(1) + U(9) \right]}$$

In essence, $K_f$ is the fraction of filterable flow to the dregs filter which is recovered. In terms of mill performance this split coefficient is a measure of the efficiency of the dregs filter and thus could be used to determine when the filter belt should be cleaned.

Using the above definition for the split parameter of the dregs filter, the following set of definitions for the state of the GLC module can be derived.
\( \text{Na}_2\text{CO}_3: \quad XG(1) = \frac{YF(1)}{1-K_f(1-\eta_{\text{glc}})} \) \hfill (111)

\( \text{Na}_2\text{S}: \quad XG(2) = \frac{YF(2)}{1-K_f(1-\eta_{\text{glc}})} \) \hfill (112)

\( \text{Na}_2\text{SO}_4: \quad XG(3) = \frac{YF(3)}{1-K_f(1-\eta_{\text{glc}})} \) \hfill (113)

\( \text{Water:} \quad XG(4) = \frac{U(8)+K_fU(9)}{1-K_f(1-\eta_{\text{glc}})} \) \hfill (114)
CAUSTICIZING AND CALCINING MODULE

The causticizing and calcining module cannot be reformulated into an explicit set of equations as was previously done for the evaporator, furnace and green liquor clarification modules. The reason for this difference is due to the complexity involved in solving the kiln model, which requires the integration of eight nonlinear first order differential equations. However, the models for this portion of the kraft mill have been rewritten in terms of a state vector and control vector with some resulting simplifications.

VARIABLE DEFINITIONS

The state vector for the causticizing module is defined as

\[
X_C = \begin{bmatrix}
X_C(1) \\
X_C(2) \\
X_C(3) \\
X_C(4) \\
X_C(5) \\
X_C(6) \\
X_C(7)
\end{bmatrix} = \begin{bmatrix}
W_L x_{Na_2CO_3}^C \\
W_L x_{Na_2S}^C \\
W_L x_{Na_2SO_4}^C \\
W_L x_w^C \\
W_L x_{NaOH}^C \\
W_L x_{Ca(OH)_2}^C \\
W_L x_{CaCO_3}^C
\end{bmatrix}
\] (115)

which represents the seven components which make up the white liquor and lime mud slurry flowing from the causticizing tanks. The units are lb/tadp.
The state of the white liquor filter relating the lime mud slurry and the flow to the digester is defined as

\[
XWLC = \begin{bmatrix}
XWLC(1) \\
XWLC(2) \\
XWLC(3) \\
XWLC(4) \\
XWLC(5)
\end{bmatrix} = \begin{bmatrix}
W_{wlf}(wlf) \times (wlf) \\
W_{wlf}(wlf) \times (wlf) \\
W_{wlf}(wlf) \times (wlf) \\
W_{wlf}(wlf) \times (wlf) \\
W_{wlf}(wlf) \times (wlf)
\end{bmatrix}
\tag{116}
\]

which represents the five components in the white liquor. The units are lb/tadp.

The control vector for the causticizing module is

\[
U = \begin{bmatrix}
U(10) \\
U(11) \\
U(12) \\
U(13) \\
U(14)
\end{bmatrix} = \begin{bmatrix}
y_F \times W_{gN}/N \\
W_{gN} \\
RPM \\
X_w \\
W_{wlf}
\end{bmatrix}
\tag{117}
\]

which is, in order, the fuel rate to the kiln (lb/hr), the nitrogen mass flow rate in the draft to the kiln (lb/hr), the rotational speed of the kiln (rpm), the concentration of water in the lime mud slurry to the kiln and the wash water spray to the white liquor filter (lb/tadp).
MATHEMATICAL MODEL FOR THE CAUSTICIZING MODULE

The state of the causticizing module in terms of the state notation for the GLC and causticizing modules is:

\[ \text{Na}_2\text{CO}_3: \quad \text{XC}(1) = \eta_{\text{glc}} \cdot \text{XG}(1) - 1.325 \cdot \text{XC}(5) \quad (118) \]

where the coefficient 1.325 is the ratio of the molecular weight of sodium carbonate to twice the weight of sodium hydroxide.

\[ \text{Na}_2\text{S}: \quad \text{XC}(2) = \eta_{\text{glc}} \cdot \text{XG}(2) \quad (119) \]

\[ \text{Na}_2\text{SO}_4: \quad \text{XC}(3) = \eta_{\text{glc}} \cdot \text{XG}(3) \quad (120) \]

\[ \text{Water}: \quad \text{XC}(4) = \eta_{\text{glc}} \cdot \text{XG}(4) - 0.243 \cdot R_{\text{Ca(OH)}} \quad (121) \]

The coefficient 0.243 represents the ratio of the molecular weight of water to calcium hydroxide.

\[ \text{NaOH}: \quad \text{XC}(5) = 1.081 \cdot \eta_c \cdot R_{\text{Ca(OH)}} \quad (122) \]

where \( \eta_c \) is the causticizing efficiency.

\[ \text{Ca(OH)}_2: \quad \text{XC}(6) = (1 - \eta_c) R_{\text{Ca(OH)}} \quad (123) \]

\[ \text{CaCO}_3: \quad \text{XC}(7) = R_{\text{CaCO}_3} + W_{\text{CaCO}_3}^{(k)} \quad (124) \]

where \( R_{\text{CaCO}_3} \) is the formation rate of calcium carbonate and \( W_{\text{CaCO}_3}^{(k)} \) represents the unconverted lime which is assumed returned to the slaker-classifier as calcium carbonate by the reburned lime flow.

In order to determine the amount of white liquor which is separated out of the slurry at the white liquor filter, a split
parameter is defined for each equivalent filter bed of the idealized model. The split coefficient for the first filter bed is

\[ K_f^{(1)} = \frac{W_{wlf}}{W_{w1} (1 - X_{Ca(OH)_2}^{(c)} - X_{CaCO_3}^{(c)})} \]

where the numerator is the flow of filtered white liquor from the first filter bed and the denominator represents the total white liquor flow to the filter. It is assumed that the calcium hydroxide, calcium carbonate and grits, which comprise the lime mud are completely retained on the "filter." The second split coefficient specifies the percentage of remaining white liquor which is recovered after the wash zone of the white liquor filter.

\[ K_f^{(2)} = \frac{W_{wlf}}{W_{w1} (1 - X_{Ca(OH)_2}^{(wmt)} - X_{CaCO_3}^{(wmt)})} \]

where the numerator is the flow of filtered white liquor from the second filter bed and the denominator is the total white liquor flow from the mix tank.

It is important to realize the \( K_f^{(1)} \) and \( K_f^{(2)} \) can change with each iteration of the optimization since the total filterable flow and component flows may alter as the control variables are perturbed. It would be expected that the values of the split coefficients will be maximized at the end of the optimization procedure.

Given the two split parameters, the component flow of white liquor leaving the filter and flowing to the digester can be written as follows:
\begin{align}
\text{Na}_2\text{CO}_3: \quad X\text{WLC}(1) &= \left[K_f^{(1)} + K_f^{(2)} (1 - K_f^{(1)})\right] X\text{C}(1) \\
\text{Na}_2\text{S}: \quad X\text{WLC}(2) &= \left[K_f^{(1)} + K_f^{(2)} (1 - K_f^{(1)})\right] X\text{C}(2) \\
\text{Na}_2\text{SO}_4: \quad X\text{WLC}(3) &= \left[K_f^{(1)} + K_f^{(2)} (1 - K_f^{(1)})\right] X\text{C}(3) \\
\text{Water}: \quad X\text{WLC}(4) &= \left[K_f^{(1)} + K_f^{(2)} (1 - K_f^{(1)})\right] X\text{C}(4) \\
\text{NaOH}: \quad X\text{WLC}(5) &= \left[K_f^{(1)} + K_f^{(2)} (1 - K_f^{(1)})\right] X\text{C}(5)
\end{align}

The total amount of lime addition to the slaker-classifier is based on the amount of sodium carbonate in the green liquor.

\[ W_{\text{CaO}} = 0.528 \cdot \eta_{\text{glc}} \cdot X_{\text{G}}(1) \]  

where the coefficient 0.528 is the ratio of the molecular weight of lime to sodium carbonate. The amount of new lime added is the difference between the amount required by Equation 132 and the amount of reburned lime produced by the kiln.

\[ W_{\text{n1}} = W_{\text{CaO}} - W_{\text{r1}} \]  

The amount of reburned lime produced by the kiln is

\[ W_{\text{r1}} = W_b X_{\text{CaO}}^{(k)} \]  

where \( W_b \) is the calcinable mass flow rate to the kiln as calcium oxide. \( X_{\text{CaO}}^{(k)} \) is the fractional lime conversion.

The amount of calcium carbonate in the reburned lime is defined as

\[ W_{\text{CaCO}_3}^{(k)} = 1.786 W_b \left(1 - X_{\text{CaO}}^{(k)}\right) \]
where the constant 1.786 is the ratio of the molecular weight of calcium carbonate to calcium oxide.

This completes the equations given in this section for the steady-state description of the kraft recovery cycle which was used in the optimization and control work.
LIST OF SYMBOLS USED

All variable names referring to concentrations, flow rates, parameters and temperatures are subscripted and/or superscripted. The subscript indicates the physical component to which the variable name refers; the superscript specifies the unit or section of a unit from which the physical component is exiting. For example, \( w_{bl}^{(ev)} \) is the rate \( W \) of black liquor \( bl \) flow from the multiple effect evaporators \( ev \).

In the following the main symbols are listed first, then the subscripts, and finally the superscripts. Special cases are included with the main symbols.

MAIN SYMBOLS

\[ A = \text{Area (ft}^2) \]
\[ A_f = \text{Furnace cross-sectional area (ft}^2) \]
\[ A_x = \text{Kiln cross-sectional area (ft}^2) \]
\[ ADTP = \text{Pulp production (tadp)} \]
\[ B = \text{Digester model coefficient} \]
\[ B_c = \text{Kiln calcinable burden (lb/ft)} \]
\[ B_o = \text{Digester model intercept} \]
\[ c = \text{Concentration} \]
\[ c_p = \text{Specific heat (Btu/lb-°F)} \]
\[ CMRPM = \text{Digester chip meter (rpm)} \]
\[ d_1 = \text{Fraction of liquor spray equal to or larger than 500 } \mu \text{m} \]
\[ d_2 = \text{Fraction of liquor spray equal to or smaller than 10 } \mu \text{m} \]
\[ D = \text{Digester disturbance variable} \]
f = Kiln heat transfer parameter (Btu/ft\(^2\)-°R)
F = Cost performance function ($/tadp)
FA = Furnace combustion air availability function
h = Heat transfer coefficient (Btu/ft\(^2\)-°F)
H = Enthalpy (Btu/lb)
K = Reaction constant
K\(_b\) = Brown stock washer split parameter (lb/lb)
K\(_{bsw}\) = Brown stock washer rate constant
K\(_c\) = Kiln combustion rate coefficient (lb/hr)
K\(_{CO}, K_g\) = Furnace CO formation rate coefficient
K\(_{df}\) = Dregs filter rate constant
K\(_f\) = Dregs filter split parameter (lb/lb)
K\(_{(1)}\) = Furnace oxygen deficiency parameter
K\(_{H_2O}\) = Cascade evaporator mass transfer coefficient (lb/ft\(^2\)-°F-hr)
K\(_{g(e)}\) = Cascade evaporator H\(_2\)S formation rate coefficient (lb/ft\(^2\)-hr)
K\(_{H_2S}\), K\(_7\) = Furnace H\(_2\)S formation rate coefficient
K\(_{pe}\) = Precipitator efficiency
K\(_{SO_2}, K_8\) = Furnace SO\(_2\) formation rate coefficient
K\(_w\) = Kiln drying rate parameter (lb/hr)
K\(_{wlf}\) = White liquor filter rate constant
M = Atomic or molecular weight
N = Nitrogen flow in kiln (lb/ft)
P = Pressure (psia)
PENLT = Constraint violation penalty function
PFC = Ratio of Na\(_2\)CO\(_3\) fly ash to total Na\(_2\)CO\(_3\)
PFS = Ratio of \( \text{Na}_2\text{SO}_4 \) fly ash to total \( \text{Na}_2\text{SO}_4 \) in furnace gases

\( P_{\text{Na}_2\text{S}} \) = Lb \( \text{Na}_2\text{S} \)/lb Na in black liquor

Q = Heat flow (Btu/hr)

\( Q_L \) = Heat Loss (Btu/hr)

R = Reaction rate (lb/hr)

RPM = Revolutions per minute

SE = Steam economy (lb/lb)

SULF = White liquor sulfidity (lb/lb)

T = Temperature (°F)

\( T_{\text{bl1}} \) = Spray droplet distribution parameter (°F)

\( T_{\text{bl2}} \) = Spray droplet distribution parameter (°F)

\( T_{\text{bl3}} \) = Spray droplet distribution parameter (°F)

\( T_{\text{LH}} \) = Temperature of digester lower heater (°F)

\( T_i^{(i)} \) = Temperature of black liquor flowing from \( i^{th} \) evaporator effect (°F)

u = Velocity (ft/hr)

\( u_{\text{gl}} \) = Maximum furnace primary combustion gas velocity (ft/hr)

U = Control variable

W = Mass flow (lb/hr or lb/tadp)

\( W_i^{(i)} \) = Black liquor flow to \( i^{th} \) evaporator effect (lb/hr)

\( W_o^{(i)} \) = Black liquor flow to \( i^{th} \) evaporator effect (lb/hr)

\( W_{\text{lt}} \) = Required oxygen flow for complete combustion in furnace primary zone (lb/hr)

WLEA = White liquor effective alkali (lb/gal)

X = Mass fraction, digester regression model independent variable

XC = Causticizing module state
XD = Digester module state
XE = Evaporator module state
XF = Furnace module state
XGLC = Green liquor clarification state
XWL = White liquor state to digester
XWLC = White liquor state from causticizing
Y = Output vector for digester regression model
YF = Output vector for furnace model
Z = Intermediate variable
\[ \alpha_{CO}, \alpha_9 \] = Furnace secondary zone turbulence CO generation rate coefficient (ft-sec^2/lb)
\[ \alpha_{H_2S}, \alpha_7 \] = Furnace secondary zone turbulence H_2S generation rate coefficient (ft-sec^2/lb)
\[ \alpha_{SO_2}, \alpha_8 \] = Furnace secondary zone turbulence SO_2 generation rate coefficient (ft-sec^2/lb)
\[ \beta_{CO}, \beta_9 \] = Furnace secondary zone oxygen concentration CO generation rate coefficient
\[ \beta_{H_2S}, \beta_7 \] = Furnace secondary zone oxygen concentration H_2S generation rate coefficient
\[ \beta_{SO_2}, \beta_8 \] = Furnace secondary zone oxygen concentration SO_2 generation rate coefficient
\[ \delta \] = Furnace secondary zone turbulence function (lb/ft-sec^2)
\[ \Delta \] = Furnace primary zone oxygen deficiency/excess function
\[ \Delta E \] = Activation energy (Btu/lb-mole)
\[ \Delta P \] = Pressure differential ("Hg)
\[ \epsilon \] = Emissivity
\[ \eta_c \] = Causticizing efficiency
\[ \eta_e \] = Furnace spray entrainment ratio
\[ \eta_{GLC} \] = Green liquor clarifier efficiency
\[ \eta_{ot} \] = Oxidation efficiency
\[ \eta_r = \text{Smelt reduction ratio} \]
\[ \eta_s = \text{Slaking efficiency} \]
\[ \eta_{\text{soap}} = \text{Soap production ratio} \]
\[ \eta_{(f)}^{st} = \text{Furnace energy utilization ratio} \]
\[ \rho = \text{Density (lb/ft}^3) \]

**SUBSCRIPTS**

a = Air  
ast = Available furnace energy  
b = Burden  
bl = Black liquor  
bld = Weak black liquor for dilution  
blds = Solids in "dilution" black liquor  
bldw = Water in "dilution" black liquor  
bls = Black liquor solids  
blw = Black liquor water  
bp = bypass  
c = Condensate, combustion energy  
C = Carbon  
CaO = Calcium oxide (lime)  
CaCO_3 = Calcium carbonate  
Ca(OH)_2 = Calcium hydroxide  
CH_4 = Methane  
CO = Carbon monoxide  
CO_2 = Carbon dioxide  
d = Total flow to dregs filter
dregs = Undissolved particles in green liquor
ds = Dregs undissolved solids
e = Evaporated water
f = Filtrate
fs = White liquor filter undissolved solids
f1 = First filter bed filtrate
f2 = Second filter bed filtrate
F = Fuel
g = Gas
gd = Dry gas
gl = Green liquor
gN = Nitrogen gas
G = Grits
H = Hydrogen
H2O = Water
H2S = Hydrogen sulfide
i = Index
ia = Infiltration air
I = Input
j = Index
lm = Lime mud
nl = New lime
N = Nitrogen
Na = Sodium
NaOH = Sodium hydroxide
Na2CO3 = Sodium carbonate
Na2CO3f = Sodium carbonate fly ash
\( \text{Na}_2\text{CO}_3 \) = Sodium carbonate particulates
\( \text{Na}_2\text{S} \) = Sodium sulfide
\( \text{Na}_2\text{SO}_4 \) = Sodium sulfate
\( \text{Na}_2\text{SO}_4f \) = Sodium sulfate fly ash
\( \text{Na}_2\text{SO}_4p \) = Sodium sulfate particulates
\( o \) = Output
\( o_2 \) = Oxygen
\( p \) = Total pulp flow from digester
\( pf \) = Pulp fiber
\( ps \) = Dissolved solids in pulp flow
\( rl \) = Reburned lime
\( \text{RSH} \) = Methyl mercaptain \((\text{CH}_3\text{SH})\)
\( \text{RSR} \) = Dimethyl sulfide \((\text{CH}_3\text{SCH}_3)\)
\( \text{RSSR} \) = Dimethyl disulfide \((\text{CH}_3\text{S} \cdot \text{SCH}_3)\)
\( s \) = Solid mass to kiln
\( sb \) = Brown stock washer undissolved solids
\( sc \) = Salt cake \((\text{Na}_2\text{SO}_4)\)
\( sm \) = Smelt
\( smf \) = Smelt fusion
\( st \) = Steam
\( S \) = Sulfur
\( \text{SO}_2 \) = Sulfur dioxide
\( v \) = Cascade evaporator vat, water vapor
\( w \) = Water, interior kiln wall
\( w' \) = Exterior kiln wall
\( wc \) = Wood chips
wh = Cascade evaporator wheel
wl = White liquor

SUPERSCRIPSTS

bmt = Brown stock washer mix tank
bsw = Brown stock washer
bt = Blow tank
c = Causticizing tanks
cb = Char bed
ce = Cascade evaporator
cm = Reacting char
cf = Condensate flash tank
d = Digester
df = Dregs filter
dmt = Dregs filter mix tank
ev = Multiple effect evaporators
f = Filtrate
fl = First filter bed filtrate
f2 = Second filter bed filtrate
fbl = First filter bed
fb2 = Second filter bed
gece = Gas from cascade evaporator
glc = Green liquor clarifier
gpr = Gas from precipitator
g1 = Gas from primary zone
g2 = Gas from secondary zone
g5 = Gas from economizer zone
h = Black liquor heater
i = Index
k = Kiln
l = Liquid water
lm = Lime mud
ot = Oxidation tower
pe = Primary zone entrainment
pr = Precipitator
pt = Product flash tank
sdt = Smelt dissolving tank
sm = Smelt
sp = Spray nozzles
v = Water vapor
wlf = White liquor and lime mud filter
wmt = White liquor filter mix tank
1 = First parameter, primary zone
2 = Second parameter, secondary zone
5 = Economizer zone
REFERENCES CITED


SECTION IV

A KINETIC AND DYNAMIC MATHEMATICAL
MODEL OF THE KAMYR DIGESTER

Proper application of computer control to the Kamyr digester as in all industries, demands the development of an accurate yet relatively simple mathematical model of the process. The model must encompass aspects of both the dynamic and the chemical kinetic behavior of the continuous digester to be properly applicable.

Because of the distributed nature of the operation of the digester, the lengthwise nature of the temperature and flow variables imposed, and the very complex form of the chemical compounds involved, this has proven to be a difficult task. Recent developments in kinetic analysis techniques, the use of hybrid computers, and the availability of more complete plant data has eased this task somewhat. This study takes advantage of the above to present a new model which appears to more correctly represent the behavior of the Kamyr digester and particularly the chemical reactions occurring therein than any previous model available in the literature.
THE KINETIC MODEL

Attempts to elucidate the kinetics of the delignification of wood to produce a pulp suitable for papermaking have been a very popular paper industry research topic. Both Rydholm (11) and Kleppe (9) have given extensive discussions of the most important of these. Suffice it to say here that the vast majority of these (particularly the earlier ones) have been severely handicapped by a lack of sufficient intermediate chemical analysis data and of knowledge of lignin polymer. Details of the latter are still not completely available but Rydholm ((11), p191) summarizes that which is presently known. Previous work has, however, listed a set of details of the behavior of the process which must be accounted for by any kinetic model attempting to explain the reaction. These are presented in Table I.

The mechanism of lignin polymer linkage fracture chosen for use in this analysis is that attributed to Ashorn (1) and Enkvist (3) as discussed by Rydholm ((11), p205-207, 594-596) and further explained by Falkehag (4).

Figure 2 presents pertinent information from Rydholm's discussion ((11), p191) to help explain this mechanism and the important reaction steps involved. The presence of a phenolic bond in the 4th position on the aromatic nucleus of the molecule promotes either the severance of the β aryl ether bond with alkali directly or the substitution of SH⁻ for OH⁻ at the α position with subsequent severance of the β aryl ether bond as in Equations 1 and 2. Note that either reaction makes available an additional phenolic site to promote further reaction.
TABLE I

LIST OF CHARACTERISTICS OF THE CHEMISTRY
OF THE KRAFT PULPING PROCESS
PERTINENT TO MATHEMATICAL MODELS
OF ITS KINETICS (2,7,9,10,11,12)

1. The reaction will proceed with or without the addition
   of sulfide to the hydroxide reagent.

2. The addition of sulfide appears to speed up the over-
   all reaction by a factor of about three with equal
   effects on lignin removal and on overall "yield."

3. It appears that there are at least two distinct
   rates of reaction in the delignification process.
   Researchers have often treated these in the past as
   the successive reactions of two distinct species.

4. In addition to the two distinct finite rates there
   appears to be a set of "extractive" materials which
   are removed very rapidly at the start of the reaction.

5. Degradation of carbohydrate materials also appears
   to follow a multiple reaction mechanism.
FIGURE 1
KAMYR DIGESTER - CONTINUOUS COOKING PROCESS

ZONES
A. IMPREGNATION
B. HEATING
C. COOKING
D. QUENCH
E. WASHING
F. COOLING

STREAMS
1. FEED
2. UPPER COOK
3. LOWER COOK
4. SECONDARY
5. SPENT LIQUOR
6. QUENCH
7. WASH
8. FILTRATE
9. BLOW
FIGURE 2

PERTINENT COMPONENTS OF THE BASIC LIGNIN MICROMOLECULE
The two different rates of reaction mentioned earlier (8,10) can be explained by noting on Figure 2 the fact that an ether bond also occurs on the γ position (L₂) in a ratio of 27/62 of those on the β position (1) or approximately 30% of the cases if it is assumed that they do not occur together for stearic reasons. Reaction would proceed in the same way as in Equations (1) and (2)
above except at a lower rate due to the lower reactivity of the γ position in comparison to the β position.

Analysis of the kinetic data available to us, that of Daleski (2) and that obtained from the WESTVACO Company (4) and Table II, indicated a strong dependence in both Equations 1 and 2 on hydroxide, OH⁻, concentration. The data also indicated a major influence of sulfur (taken as SH⁻) but there was not sufficient variation in sulfur levels to completely clarify this dependence. Hence it was treated as a catalytic type reaction.

Daleski (2) presents several groupings of the carbohydrate components of wood. We were able to get the best fit by using the three components: cellulose, C₁; galactoglucomannan, C₂; and araboylan, C₃. Table III presents the initial values for these as derived from Daleski's data (2) and inferred for the WESTVACO data (4) from information in Rydholm (11, p.97). For the same reasons as above each of these were assumed to be attacked by either OH⁻ or SH⁻ in combination.

The overall reactions are then as follows:

\[
\begin{align*}
L₁ + OH⁻ & \xrightarrow{k₁} \text{soluble products} \\
L₁ + OH⁻ & \xrightarrow{k₂} \text{soluble products} \\
L₂ + OH⁻ & \xrightarrow{k₃} \text{soluble products} \\
L₂ + OH⁻ & \xrightarrow{k₄} \text{soluble products}
\end{align*}
\] (3) (4) (5) (6)
**TABLE IIA**

KINETIC DATA USED IN THE FITTING OF KINETIC COEFFICIENTS TO THE MODEL PRESENTED HEREIN (4).

<table>
<thead>
<tr>
<th>Active Alkali [gms NaOH/gm Oven Dry Wood] X 100</th>
<th>22.3</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sulfidity, [100 Na₂S/(Na₂S+NaOH)] as Sodium Equivalents</td>
<td>25.4</td>
</tr>
<tr>
<td>Liquor to Wood Ratio, Liters per Kilogram of Oven Dry Wood</td>
<td>3.5</td>
</tr>
<tr>
<td>Wood Extractives (Alcohol and Benzene Soluble) Per cent Oven Dry Wood</td>
<td>3.3</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Cook No.</th>
<th>Reaction Time(min.)</th>
<th>Temperature °C</th>
<th>Yield as % Oven Dry Wood</th>
<th>Acid Insoluble Remaining Lignin As % Oven Dry Wood</th>
</tr>
</thead>
<tbody>
<tr>
<td>---</td>
<td>0</td>
<td>80</td>
<td>100.0</td>
<td>26.4</td>
</tr>
<tr>
<td>611</td>
<td>70</td>
<td>150</td>
<td>74.5</td>
<td>20.2</td>
</tr>
<tr>
<td>612</td>
<td>75</td>
<td>155</td>
<td>73.2</td>
<td>18.95</td>
</tr>
<tr>
<td>613</td>
<td>80</td>
<td>160</td>
<td>69.9</td>
<td>16.8</td>
</tr>
<tr>
<td>614</td>
<td>85</td>
<td>165</td>
<td>68.3</td>
<td>15.3</td>
</tr>
<tr>
<td>615</td>
<td>90</td>
<td>170</td>
<td>65.4</td>
<td>14.1</td>
</tr>
<tr>
<td>621</td>
<td>105</td>
<td>170</td>
<td>60.7</td>
<td>10.3</td>
</tr>
<tr>
<td>616</td>
<td>120</td>
<td>170</td>
<td>55.0</td>
<td>7.5</td>
</tr>
<tr>
<td>617</td>
<td>150</td>
<td>170</td>
<td>49.9</td>
<td>4.75</td>
</tr>
<tr>
<td>618</td>
<td>180</td>
<td>170</td>
<td>48.3</td>
<td>3.7</td>
</tr>
<tr>
<td>619</td>
<td>240</td>
<td>170</td>
<td>46.3</td>
<td>2.1</td>
</tr>
<tr>
<td>620</td>
<td>270</td>
<td>170</td>
<td>45.4</td>
<td>1.8</td>
</tr>
</tbody>
</table>

Temperature raised linearly from 80°C at 1°C per minute during cook to maximum noted temperature then held constant for remaining time.
TABLE IIIB

KINETIC DATA USED IN THE FITTING OF KINETIC COEFFICIENTS TO THE MODEL PRESENTED HEREIN (4).

<table>
<thead>
<tr>
<th>Active Alkali [gms NaOH/gm Oven Dry Wood] X 100</th>
<th>22.6%</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sulfidity, [100 Na_2S/(Na_2S+NaOH)] as Sodium Equivalents</td>
<td>27.2%</td>
</tr>
<tr>
<td>Liquor to Wood Ratio, Liters per Kilogram of Oven Dry Wood</td>
<td>3.5</td>
</tr>
<tr>
<td>Wood Extractives (Alcohol and Benzene Soluble) Per Cent Oven Dry Wood</td>
<td>3.3</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Cook No.</th>
<th>Time(min.)</th>
<th>Temperature °C</th>
<th>Yield(%ODW)</th>
<th>Lignin(%ODW)*</th>
</tr>
</thead>
<tbody>
<tr>
<td>---</td>
<td>0</td>
<td>80</td>
<td>100.0</td>
<td>26.4</td>
</tr>
<tr>
<td>761</td>
<td>115</td>
<td>165</td>
<td>60.0</td>
<td>9.8</td>
</tr>
<tr>
<td>762</td>
<td>135</td>
<td>165</td>
<td>55.1</td>
<td>7.5</td>
</tr>
<tr>
<td>763</td>
<td>175</td>
<td>165</td>
<td>50.5</td>
<td>5.25</td>
</tr>
<tr>
<td>764</td>
<td>255</td>
<td>165</td>
<td>47.0</td>
<td>7.8</td>
</tr>
</tbody>
</table>

*Not determined directly but calculated from previous data.

Same temperature profile as Table IIA.
TABLE IIC

KINETIC DATA USED IN THE FITTING OF KINETIC COEFFICIENTS TO THE MODEL PRESENTED HEREIN (4).

<table>
<thead>
<tr>
<th>Active Alkali [gms NaOH/gm Oven Dry Wood] X 100</th>
<th>20.9%</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sulfidity, [100 Na₂S/(Na₂S+NaOH)] as Sodium Equivalents</td>
<td>27.2%</td>
</tr>
<tr>
<td>Liquor to Wood Ratio, Liters per Kilogram of Oven Dry Wood</td>
<td>3.5</td>
</tr>
<tr>
<td>Wood Extractives (Alcohol and Benzene Soluble) Per Cent Oven Dry Wood</td>
<td>3.3</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Cook No.</th>
<th>Time(min.)</th>
<th>Temperature°C</th>
<th>Yield(%ODW)</th>
<th>Lignin(%ODW)*</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>0</td>
<td>80</td>
<td>100.0</td>
<td>26.4</td>
</tr>
<tr>
<td>757</td>
<td>120</td>
<td>170</td>
<td>58.6</td>
<td>8.34</td>
</tr>
<tr>
<td>758</td>
<td>140</td>
<td>170</td>
<td>53.1</td>
<td>6.48</td>
</tr>
<tr>
<td>759</td>
<td>180</td>
<td>170</td>
<td>48.8</td>
<td>4.15</td>
</tr>
<tr>
<td>760</td>
<td>260</td>
<td>170</td>
<td>46.4</td>
<td>2.23</td>
</tr>
</tbody>
</table>

*Not determined directly but calculated from previous data.

Same temperature profile as Table IIA.
TABLE IID

KINETIC DATA USED IN THE FITTING OF KINETIC COEFFICIENTS TO THE MODEL PRESENTED HEREIN (4).

| Active Alkali, [gms NaOH/gm Oven Dry Wood] X 100 | 19.5% |
| Sulfidity, [100 Na₂S/(Na₂S+NaOH)] as Sodium Equivalent | 27.2% |
| Liquor to Wood Ratio, Liters per Kilogram of Oven Dry Wood | 3.5 |
| Wood Extractives (Alcohol and Benzene Soluble) Per Cent Oven Dry Wood | 3.3 |

<table>
<thead>
<tr>
<th>Cook No.</th>
<th>Time(min.)</th>
<th>Temperature°C</th>
<th>Yield(%ODW)</th>
<th>Lignin(%ODW)*</th>
</tr>
</thead>
<tbody>
<tr>
<td>---</td>
<td>0</td>
<td>80</td>
<td>100.0</td>
<td>26.4</td>
</tr>
<tr>
<td>756</td>
<td>180</td>
<td>170</td>
<td>47.9</td>
<td>3.4</td>
</tr>
<tr>
<td>766</td>
<td>180</td>
<td>170</td>
<td>47.9</td>
<td>3.6</td>
</tr>
<tr>
<td>765</td>
<td>270</td>
<td>170</td>
<td>45.2</td>
<td>1.7</td>
</tr>
<tr>
<td>767</td>
<td>270</td>
<td>170</td>
<td>44.6</td>
<td>1.5</td>
</tr>
</tbody>
</table>

*Not determined directly but calculated from previous data.

Same temperature profile as Table IIA.
TABLE III

ESTABLISHMENT OF INITIAL COMPONENT VALUES
OF TEST DATA

<table>
<thead>
<tr>
<th></th>
<th>DALESKI(2)</th>
<th>WESTVACO(4)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1. As Reported in the Literature</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Lignin</td>
<td>% 29.10</td>
<td>26.4</td>
</tr>
<tr>
<td>Glucose</td>
<td>% 45.53</td>
<td>---</td>
</tr>
<tr>
<td>Mannose</td>
<td>% 9.85</td>
<td>---</td>
</tr>
<tr>
<td>Xylose</td>
<td>% 6.56</td>
<td>---</td>
</tr>
<tr>
<td>Arabinose</td>
<td>% 1.39</td>
<td>---</td>
</tr>
<tr>
<td>Alcohol/Benzene</td>
<td>% 3.50</td>
<td>3.3</td>
</tr>
<tr>
<td>Extractives</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Total</td>
<td>95.94</td>
<td></td>
</tr>
</tbody>
</table>

2. Normalized for Use Here

|                  |            |             |
| Lignin           | % 29.10    | 26.4 Measured |
| Glucose          | % 48.50    | 52.6+        |
| Mannose          | % 10.45    | 10.2*        |
| Xylose           | % 6.97     | 6.5*         |
| Arabinose        | % 1.48     | 1.0*         |
| Alcohol/Benzene  | % 3.50     | 3.3 Measured |
| Extractives      |             |             |
| Total            |             |             |

3. As Used

|                  |            |             |
| Lignin, $L_1$    | % 20.37    | 18.48       |
| Lignin, $L_2$    | % 8.73     | 7.52        |
| Cellulose, $C_1$ | % 44.32    | 48.52       |
| (Glucose-0.4 (Mannose)) | | |
| Galactoglucomman, $C_2$ | % 14.63    | 14.28       |
| (1.4(Mannose))   |            |             |
| Araboxylan, $C_3$| % 7.73     | 7.22        |
| (1.11(Xylose))   |            |             |

The latter two are considered Hemicelluloses.
*Derived from Rydholm (11), p 97.
+Glucose was obtained by difference.
\[ C_1 + OH^- \rightarrow \text{degradation products} \quad (7) \]
\[ C_1 + OH^- \rightarrow \text{degradation products} \quad (8) \]
\[ C_2 + OH^- \rightarrow \text{degradation products} \quad (9) \]
\[ C_2 + OH^- \rightarrow \text{degradation products} \quad (10) \]
\[ C_3 + OH^- \rightarrow \text{degradation products} \quad (11) \]
\[ C_3 + OH^- \rightarrow \text{degradation products} \quad (12) \]
\[ \text{Na}_2S + H_2O \rightarrow 2\text{Na}^+ + OH^- + SH^- \quad (13) \]

Each reaction coefficient \( k_i \) was expressed in the Arrhenious form:
\[ k_i = A_i e^{-E_i/RT} \quad (14) \]

Differential equations written for each reaction above were then solved on the hybrid computer for fitting the kinetic coefficients against both literature data (2,12) and new laboratory data (4) supplied by the WESTVACO Company and presented in Table II. Results of these fits are given in Figures 3-6 and Table IV. Note that \( OH^- \) and \( SH^- \) compositions are given for the WESTVACO run, Figure 6. These values are essentially constants for the Daleski data (2).

The \( \alpha \) hydroxyl group in lignin is present in only 20% of the cases. However, a \( \gamma \) hydroxyl group is present in at least 70% of
FIGURE 3
COMPARISON OF EXPERIMENTAL AND SIMULATED KINETIC DATA FOR KRAFT PULPING DATA OF DALESKI (2) AT 180°C.
FIGURE 4

COMPARISON OF EXPERIMENTAL AND SIMULATED KINETIC DATA FOR KRAFT PULPING
DATA OF DALESKI (2) AT 195°C
COMPARISON OF EXPERIMENTAL AND SIMULATED KINETIC DATA FOR SODA PULPING DATA OF DALESKI (2) AT 195°C

FIGURE 5

YIELD %

TIME (MINUTES)

100 80 60 40 20 0

0 15 12 9 6 3 0

30 24 18 12 6

AMOUNT REMAINING %
FIGURE 6
COMPARISON OF EXPERIMENTAL AND SIMULATED
KINETIC DATA FOR KRAFT PULPING
DATA OF WESTVACO (TABLE IIIB)(4)
TABLE IV

VALUES OF A AND E IN THE ARRHENIUS EXPRESSION FOR THE KINETIC MODEL OF THE KRAFT PULPINGREACTION

\[ k_i = A_i e^{-E_i/RT} \left([g/(L)(min.)]^{-1}\right) \]

<table>
<thead>
<tr>
<th>k</th>
<th>A</th>
<th>E</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>3.6 x 10^{11}</td>
<td>30,000</td>
</tr>
<tr>
<td>2</td>
<td>3.0 x 10^{09}</td>
<td>26,000</td>
</tr>
<tr>
<td>3</td>
<td>2.9 x 10^{08}</td>
<td>25,000</td>
</tr>
<tr>
<td>4</td>
<td>1.1 x 10^{09}</td>
<td>25,000</td>
</tr>
<tr>
<td>5</td>
<td>3.5 x 10^{09}</td>
<td>28,000</td>
</tr>
<tr>
<td>6</td>
<td>3.4 x 10^{10}</td>
<td>30,000</td>
</tr>
<tr>
<td>7</td>
<td>3.4 x 10^{10}</td>
<td>29,000</td>
</tr>
<tr>
<td>8</td>
<td>3.8 x 10^{10}</td>
<td>29,000</td>
</tr>
<tr>
<td>9</td>
<td>2.1 x 10^{11}</td>
<td>30,000</td>
</tr>
<tr>
<td>10</td>
<td>1.8 x 10^{11}</td>
<td>30,000</td>
</tr>
</tbody>
</table>
the cases. It can be assumed that these latter supply the necessary reactive sites for alkyl aryl ether bond breakage required to completely break down the lignin polymer.

As can be seen from Figures 3-6 this mechanism does give a satisfactory fit to the available data on loblolly pine. It must of course be refitted to data for other wood species as these become available.
DIGESTER DYNAMIC MODELS

In order to be useful for computer control, dynamic models of plant components must be kept as simple as possible while still being consistent with reality and the necessity to adequately describe the behavior observed. In order to accomplish this in the case of the continuous digester the set of assumptions listed in Table V has been adopted. The resulting model is as follows:

\[
\frac{dl}{dt} = f(F_w, F_R, l) \tag{15}
\]

\[
\frac{dT}{dl} = f \left( \frac{F_H}{\left[ F_H + (F_w + F_R) \right]} \right) (T_R - T) \tag{16}
\]

\[
\frac{dT}{dt} = \frac{dT}{dl} \cdot \frac{dl}{dt}
\]

\[
\frac{dL_1}{dt} = - k_1(L_1)(OH^-) - k_2(L_1)(SH^-)(OH^-) \tag{17}
\]

\[
\frac{dL_2}{dt} = - k_3(L_2)(OH^-) - k_4(L_2)(SH^-)(OH^-) \tag{18}
\]

\[
\frac{dC_1}{dt} = - k_5(C_1)(OH^-) - k_6(C_1)(SH^-)(OH^-) \tag{19}
\]

\[
\frac{dC_2}{dt} = - k_7(C_2)(OH^-) - k_8(C_2)(SH^-)(OH^-) \tag{20}
\]

\[
\frac{dC_3}{dt} = - k_9(C_3)(OH^-) - k_{10}(C_3)(SH^-)(OH^-) \tag{21}
\]
TABLE V

ASSUMPTIONS MADE IN DERIVING THE KINETIC AND DYNAMIC MODEL OF THE KAMYR CONTINUOUS DIGESTER FOR THE KRAFT PULPING PROCESS

1. The relationship between the distance from the top of the digester and the retention time is a known function of the flow rates in the digester.

2. The flow of chips through the digester is of plug-flow type.

3. Permeation of reactant fluid throughout the chip is considered fast compared to the reaction time, thus wood diffusion effects are considered negligible.

4. The downward movement of free liquor in the upper part of the digester is of the plug type, i.e., there is no axial diffusion of material or energy but full radial mixing of both.

5. The upward movement of the washing liquor in the washing zone is also of the plug type.

6. Chips in the cooking zone are considered to be at the same temperature as their environmental conditions. There are no temperature gradients in the chips themselves.

7. Wood is regarded as a homogeneous mixture of its various components for the purpose of these reaction calculations.
TABLE V (Continued)

8. Wood is considered to be composed of three major substances, lignin, hemicelluloses and cellulose. Extractants are considered to have been removed prior to any major reaction taking place.

9. Effective alkali is an adequate measure of the hydroxyl ion concentration in the cooking liquor.

10. Effective sulfidity is an adequate measure of the $\text{SH}^-$ ion concentration in the cooking liquor.

11. The lignin content calculated with the weight of dry wood as a basis may be used as a measure of lignin "concentration."

12. No lignin condensation reactions occur.

13. Temperature gradients in heating, and quench zones are considered to be linear with driving force throughout the length of each pertinent zone. There are no radial gradients.
Yield \quad = \quad L_1 + L_2 + C_1 + C_2 + C_3 \quad (22)

L_{1\text{init.}} \quad = \quad (0.70) \text{ (Total Lignin)} \quad (23)

L_{2\text{init.}} \quad = \quad (0.30) \text{ (Total Lignin)} \quad (24)

Kappa Number = \frac{(L_1 + L_2)}{(0.153)(\text{Yield})} \quad (25)

The general countercurrent flow equations of the wash zone give for the temperature distribution:

\rho_1 A c_v c_p \frac{\partial T_1}{\partial x} = U A_w (T_1 - T_2) \quad (26a)

Collecting terms:

v_1 \frac{\partial T_1}{\partial x} = K (T_1 - T_2) \quad (26b)

and

\frac{\partial T_1}{\partial x} = \frac{K}{v_1} (T_1 - T_2) \quad (26c)

likewise

\frac{\partial T_2}{\partial x} = - \frac{K}{v_1} (T_2 - T_1) \quad (26d)

A similar equation for black liquor solids distribution gives:

\frac{\partial S_1}{\partial x} = \frac{K}{v_1'} (S_1 - S_2) \quad (27a)

and

\frac{\partial S_2}{\partial x} = - \frac{K}{v_2'} (S_2 - S_1) \quad (27b)
The reader should note from Figure 1 that the flow of pulp and of wash liquor is countercurrent in the wash zone while the wood chip and reactant flow is concurrent in the reaction zones. This necessitates treating the total computations in two separate parts on the hybrid computer.
APPLICATION TO CONTROL STUDIES

Figure 7 presents a typical temperature profile and resulting reaction and yield curve for the reaction zone of a Kamyr digester as produced by this study. Figures 8-9 show the corresponding temperature and solids content curves for the washing zone of the same digester.

Because of the plug flow nature of the model, it must be used repeatedly in the off-line mode to determine a complete set of responses to possible upsets and changes. These can then be cross-correlated to obtain an algebraic steady state equation which can predict the result of any suggested upset or control change.

The strong dependence of reaction rates on hydroxide concentration suggest the possibility of making effective use of the intermediate addition of fresh alkali in the digester as a reaction control mechanism along with the present temperature profile method.
FIGURE 7
TYPICAL PROFILES FOR KAMYR DIGESTER
REACTION ZONE
INITIAL CONDITIONS SAME AS IN TABLE IIB
CASE 1 - WASH FLOW = DOWN FLOW
CASE 2 - WASH FLOW = 2 (DOWN FLOW)

FIGURE 8
SAMPLE WASH ZONE - TEMPERATURE PROFILES
CASE 1 - WASH FLOW = DOWN FLOW
CASE 2 - WASH FLOW = 4 (DOWN FLOW)

\[ \frac{K}{v_1} = 4 \]

FIGURE 9
SAMPLE WASH ZONE - COMPOSITION PROFILES
LIST OF SYMBOLS USED

A = Area of heat or mass transfer
A_i = Frequency factor in the Arrhenius expression
A_c = Cross-sectional area of digester
a = A constant
C_i = Effective concentration of cellulose (glucose -0.4 (Mannose))
C_2 = Effective concentration of galacloglucommans, GGM (1.4(Mannose))
C_3 = Effective concentration of araboxylan; (1.11(Xylose))
CMRPM = Chip meter RPM
CMVOL = Chip meter volume per RPM
c = Heat capacity of dry wood
E_i = Activation energy factor in the Arrhenius expression
EA/W = Effective alkali to wood ratio
F = Flow rates
H_i = As subscript refers to heater location
H_{SV} = Heat content difference between steam and condensate at steaming vessel conditions
j = As subscript refers to heater location
K = Heat transfer factor
K = Diffusion factor
k_i = A reaction coefficient
L_1 = Effective concentration of lignin with β aryl ether bonds
L_2 = Effective concentration of lignin with γ alkyl ether bonds.
m = Moisture fraction of wet chips
OH^- = Effective concentration of hydroxyl ion
Overscore  = Nominal value
R          = Gas constant
            As subscript pertains to reactant flow.
S          = Black liquor solids concentration
SH⁻        = Effective concentration of bisulfide ion
T          = Absolute temperature
T_{amb}    = Ambient temperature
t_{blow}   = Blow pulse duration
T_{wash}   = Temperature set point of wash heater
T_{LHSP}   = Lower heater temperature set point
T_{SV}     = Steaming vessel temperature
T_i        = Temperature at specified location
t          = Time
t_R        = Residence time from lower heater to blow line
Underscore = Indicates a vector quantity
v_i        = Fluid velocity
v'_i       = Velocity factor for heat transfer
v''_i      = Velocity factor for mass transfer
W          = As subscript refers to wood chip
W_{blow}   = Blow flow
\Delta W_{blow} = Nominal blow flow change for level control
W_{dil}    = Dilution flow (water fed other than white liquor)
W_{bypass} = Bypass filtrate flow
W_{ext}    = Extraction flow
W_{PulpSP} = Required pulp production rate
W_{wd}     = Wet wood feed rate
\( W_{WL} \) = White liquor flow rate

\( X \) = Position as regards normalized length

\( X_{\text{lig}} \) = Ratio of lignin/pulp set point

\( X_{\text{pulp}_{SP}} \) = Consistency of blow flow

\( X_{\text{pulp}} \) = Fully diluted initial concentration of effective alkali

\( X_{\text{SH}} \) = Fully diluted concentration of sodium hydrosulfide

\( X_{\text{OH}} \) = White liquor effective alkali concentration

\( X_{\text{WL}} \) = White liquor fully hydrolyzed sodium hydrosulfide concentration

\( \text{Yield} \) = Expected yield (from model)

\( \Delta \) = As prefix indicates change in

\( \rho_{BD} \) = Chip density

\( \rho_{BD}' \) = New chip density

\( \rho_{BD}'\) = New desired value
REFERENCES CITED


SECTION V
A DYNAMIC MODEL OF THE MULTIPLE EFFECT EVAPORATORS

In this section, a linear, lumped, dynamic mathematical model for the long-tube vertical black liquor evaporator is derived on the basis of the physical processes taking place in the various portions of an evaporator. The model is then simplified by replacing some of the dynamic equations which have very small time constants by algebraic equations. The model was then set up for the sextuple-effect evaporator system with parallel feed to the Fifth and Sixth Effects as shown in Figure 1.
FIGURE 1
FLOW DIAGRAM FOR SEXTUPLE-EFFECT BLACK LIQUOR EVAPORATOR SYSTEM
AT CONSOLIDATED PAPERS, INC., WISCONSIN RAPIDS, WISCONSIN
PHYSICAL PROCESSES IN AN EVAPORATOR

For the purpose of modelling, the long-tube vertical evaporator is divided into the following parts [1]:

A. Main liquor box
B. Non-boiling tube section
C. Boiling tube section
D. Steam chest
E. Vapor space

MAIN LIQUOR BOX

The main liquor box is physically the lowest portion of an LTV evaporator. The black liquor which is pumped into it under pressure, rises through the tubes of the non-boiling section. The dynamic effects present are contributed by the mixing which occurs in the main liquor box. Weak black liquor enters the box at a velocity of about 4 ft/sec, whereas it leaves the main liquor box at about 0.06 ft/sec. As a result, flow eddies are formed, and non-ideal mixing of black liquor takes place. The extent of this mixing depends upon the position of the liquor inlet, relative velocities of liquor flow at inlet and exit, and the interior design of the box. The time constant of mixing is taken to be a fraction (60% value in our simulation) of that for ideal mixing in a volume of the same size. A certain amount of mixing of black liquor takes place during its flow through the non-boiling section. This mixing can be combined with the mixing occurring in the main liquor box (MLB).
Mathematically, 

\[ F(t) C_{BLN}(t) - F(t) C_{BL \text{ out}, MLB}(t) \]

\[ = V_{MLB \text{ eff}} \frac{dC_{BL \text{ out}, MLB}}{dt} \]  \hspace{1cm} (1)

where \( F(t) \) is the volumetric flow rate of black liquor, and \( C_{BLN} \) and \( C_{BL \text{ out}, MLB} \) are concentrations of liquor incoming and leaving MLB. \( V_{MLB \text{ eff}} \) is the effective volume (or equivalent volume for an ideal mixer). Equation (1) can be rewritten as,

\[ \frac{dC_{BL \text{ out}, MLB}(t)}{dt} = \frac{M_{BLN}(t)}{\rho_{BLN}(t) V_{MLB \text{ eff}}} (C_{BLN}(t) - C_{BL \text{ out}, MLB}(t)) \]  \hspace{1cm} (2)

Here, \( M_{BLN} \) and \( \rho_{BLN} \) are the mass flow rate and the density respectively of the black liquor entering the main liquor box. When linearizing Equation (2) about an operating point, each variable is given as the sum of its value at an operating point (which is denoted by the overscore \( \bar{\cdot} \)), and the remaining small component (which is denoted by \( \Delta \)). The variable associated with \( \Delta \) is a function of time \( t \), and \( (t) \) will be dropped where it is not needed for clarity. Thus:

\[ C_{BL \text{ out}, MLB}(t) = \bar{C}_{BL \text{ out}, MLB} + \Delta C_{BL \text{ out}, MLB}(t) \]  \hspace{1cm} (3)

\[ C_{BLN}(t) = \bar{C}_{BLN} + \Delta C_{BLN}(t) \]  \hspace{1cm} (4)
\[ \dot{M}_{\text{BLN}}(t) = \bar{M}_{\text{BLN}} + \Delta \dot{M}_{\text{BLN}}(t) \]  

(5)

Neglecting the second-order terms (like \( \Delta \dot{M}_{\text{BLN}} \Delta C_{\text{BLN}} \)) we can write,

\[ \frac{d \Delta C_{\text{BL out, MLB}}(t)}{dt} = \frac{\dot{M}_{\text{BLN}}}{\rho_{\text{BLN}} \cdot V_{\text{MLB eff}}} (\Delta C_{\text{BLN}}(t) - \Delta C_{\text{BL out}}(t)) \]  

(6)

The time constant for the main liquor box, or \( \tau_6 \), can be written as

\[ \tau_6 = \frac{\rho_{\text{BLN}} \cdot V_{\text{MLB eff}}}{\bar{M}_{\text{BLN}}} \]  

(7)

and Equation (6) can be rewritten as,

\[ (\tau_6 \frac{d}{dt} + 1) \Delta C_{\text{BL out, MLB}}(t) = \Delta C_{\text{BLN}}(t) \]  

(8)

NON-BOILING SECTION

The liquor under pressure from the main liquor box rises up through the tubes and is heated by the surrounding steam. At the same time the static head of liquor above the tube decreases, and therefore at some point along the tube the liquor starts to boil. This is the point of maximum temperature. The region below the point where boiling occurs is known as the non-boiling section.

The velocity of black liquor is very small in the non-boiling section. A Reynolds number of about 800 is typical. Thus the flow is laminar. The flow dynamics in the non-boiling section is represented by a pure transport lag, \( T_{\text{DNBS}} \).
Mathematically,

\[ T_{DNBS} = \frac{L_N}{V_{NBS}} \]  

The length of non-boiling section, \( L_N \), is assumed to be one-fourth of total tube length for effects 2, 3, 4, 5 and 6, and \( V_{NBS} \) is the average velocity of flow in non-boiling section at the operating point. Since Effect LB operates under natural circulation, it is assumed to be completely filled with non-boiling liquor. Correspondingly Effect IA is assumed to be totally a boiling section. These are approximately equal to the expected and actually observed behavior of the liquid in these particular effects.

Transport lags due to liquor flow through the pre-heater in the effect in question, the post-heater in the previous effect, and the connecting piping, are small because of higher flow velocities. If necessary, these lags can be lumped with the transport lag in the non-boiling section. As was mentioned earlier, the mixing of black liquor in the non-boiling and pre-heater sections, the post-heater section of the previous effect, and that of the connecting piping can be lumped together with the mixing in main liquor box as one single time constant, \( \tau_6 \).

The black liquor flow is incompressible through the non-boiling section, thus a change in mass flow rate of black liquor into the non-boiling section is felt without any delay throughout the section. However, the concentration of black liquor is related by the equation

\[ C_{BL \ out, \ MLB(t - T_D)} = C_{BL \ out, \ NBS(t)} \]
because of the time delay, $T_D$, involved. This equation can be written about the operating point as,

$$
\Delta C_{\text{BL out}} \cdot \text{MLB}(t-T_D) = \Delta C_{\text{BL out}} \cdot \text{NBS}(t)
$$

(11)

where $C_{\text{BL out}} \cdot \text{NBS}$ is the concentration of black liquor coming from the non-boiling section.

**BOILING SECTION**

The weak black liquor is heated by heat transfer through tube walls from the surrounding steam. As the liquor rises in the boiling section, the pressure is reduced, the boiling point decreases and vigorous boiling takes place. Depending on the rate of vapor bubble formation, the liquor-steam mixture is pushed through the boiling section at high velocity. The average velocity of this two-phase flow is much larger than that in the non-boiling section, and as a result the time the liquor spends in the boiling section is only about 6 seconds, compared to approximately 150 seconds in the non-boiling section. Thus it seems a reasonable simplification to neglect the retention time of the steam in the boiling section.

The material balance for solids in the boiling section is,

$$
C_{\text{BL out}} \cdot \text{NBS}(t) \cdot \dot{M}_{\text{BLN}}(t) = C_{\text{BLO, BS}}(t) \cdot \dot{M}_{\text{BLO, BS}}(t)
$$

(12)

where $C_{\text{BLO, BS}}$ and $\dot{M}_{\text{BLO, BS}}$ are concentration and mass flow rate
of black liquor leaving the boiling section.

STEAM CHEST

The steam in the steam chest condenses on the outside of the tubes for the non-boiling and boiling sections. In the process, the latent heat of vaporization is transferred through the tube wall to heat the black liquor and convert part of it into vapor. It is assumed that the steam in the steam chest is saturated, and the condensate hold-up is negligible.

A material balance equation for steam and condensate can be written as,

$$\frac{dV_{STCH}}{dt} = \dot{M}_{HSTCH} - \dot{M}_{\text{cond}}$$  \hspace{1cm} (13)

or,

$$V_{STCH} \frac{dP_{HSTCH}}{dt} = \dot{M}_{HSTCH} - \dot{M}_{\text{cond}}$$  \hspace{1cm} (14)

where

$$\dot{M}_{HSTCH} = \text{Mass flow rate of steam in steam chest}$$

$$\dot{M}_{\text{cond}} = \text{Mass rate of condensate formed}$$

$$P_{HSTCH} = \text{Pressure in steam chest}$$

$$V_{STCH} = \text{Volume of steam chest}$$

$$\rho_V = \text{Density of vapor in steam chest}$$

$$\frac{d\rho_V}{dP_{HSTCH}}$$ is estimated by $$\frac{\Delta\rho_V}{\Delta P_{HSTCH}}$$ for small deviations about
the operating point. Equation (14) can be written as

$$KVSTCH \ s \ \Delta P_{HSTCH} = \Delta \dot{M}_{HSTCH} - \Delta \dot{M}_{cond}$$

(15)

where

$$KVSTCH = \frac{APV}{\Delta P_{HSTCH}} V_{STCH}$$

(16)

and s is equivalent to $\frac{d}{dt}$. This dynamic component represented by block $P_2$ in Figure 2.

For small deviations from the operating point, the relation between saturation temperature, $T_{HSTCH}$, and saturation pressure, $P_{HSTCH}$, for steam can be approximated by the linear relation:

$$\Delta T_{HSTCH} = P_3 \ \Delta P_{HSTCH}$$

(17)

where,

$$P_3 = \frac{\Delta T_{HSTCH}}{\Delta P_{HSTCH}}$$

(18)

Since the time constant for heat transfer through the tube walls is only about 1.5 seconds, the dynamics of the tube wall is ignored in writing an energy balance equation for steam and black liquor. Total heat, $\dot{Q}_{HST}$, given by the steam equals the sum of the heat loss, $\dot{Q}_L$, to the surroundings and the heat, $\dot{Q}_T$, transferred to the black liquor. That is:

$$\dot{Q}_{HST} = \dot{M}_{cond} \gamma_{cond \ steam} = \dot{Q}_L + U_TAS \ (T_{HSTCH} - T_{BLO})$$

(19)
FIGURE 2

DETAILED LINEAR DYNAMIC MODEL FOR MULTIPLE-EFFECT EVAPORATORS

NOTE: THE RESPONSES INSIDE THE BLOCKS ARE THEIR STEP RESPONSES $G_{i,j}$ AND $F_{i,j}$
where $\gamma_{\text{cond steam}}$ is the enthalpy change per unit mass of steam condensed. The heat loss, $Q_L$, and the overall heat transfer coefficient, $U_T$, can be assumed to be constants for short time-spans and small variations about the operating point. Therefore Equation (19) reduces to:

$$\Delta Q_{\text{HST}} = \Delta M_{\text{cond steam}} \gamma_{\text{cond steam}}$$

$$= U_T A_T (\Delta T_{\text{HSTCH}} - \Delta T_{\text{BLO}})$$

(20)

The temperature of the boiling black liquor, $T_{\text{BLO}}$, can be expressed as the sum of the boiling point rise, BPR, which is a function of the concentration, and the saturated vapor temperature $T_{\text{ST sat}}$ [2]. The equation for $\Delta T_{\text{BLO}}$ can then be written as:

$$\Delta T_{\text{BLO}} = \Delta T_{\text{ST sat}} + \Delta \text{BPR}$$

(21)

These equations are represented by blocks $P_2$, $P_3$, $P_4$, $P_8$, and $G_{10}$ in Figure 2.

VAPOR SPACE

Boiling black liquor and vapor from the boiling section are pushed into the vapor space. The steam vapor flows back to the steam chest of the preceding evaporator, while the liquor is fed forward to the next stage. It is assumed here that there is no retention of black liquor in the vapor space. Let $C_{\text{BLO}}$, $M_{\text{BLO}}$, and $M_{\text{ST impressed}}$ be the concentration of black liquor, the mass flow rate of black liquor, and the mass flow rate of steam vapors leaving the effect. The material balance equation for solids can
be written as,

$$C_{BL\ out,\ BS(t)\ \dot{M}_{BLO},\ BS(t)} = C_{BLO(t)} \dot{M}_{BLO(t)} \quad (22)$$

where

$$\dot{M}_{BLO(t)} = \dot{M}_{BLN(t)} - \dot{M}_{ST\ impressed(t)} \quad (23)$$

This equation implies that mass flow rate throughout the evaporator changes simultaneously, i.e., plug-flow of liquid occurs. This is a useful approximation when the changes in other variables such as temperature and concentration are much less rapid.
DERIVATION OF OVERALL EQUATIONS

Equations for the mass flow rate and concentration of black liquor coming from an effect, the mass rate of steam generated, the vapor pressure in vapor space, and mass flow rate of steam into the steam chest can be derived from the equations given in the previous sub-section.

Equation (22) can be rewritten for dynamic variations as:

$$\Delta \dot{m}_{BLO}(t) = \Delta \dot{m}_{BLN}(t) - \Delta \dot{M}_{ST} \text{ impressed}(t)$$ (24)

Equations (12) and (22) give

$$C_{BL\text{ out, NBS}(t)} \dot{m}_{BLN}(t) = C_{BLO}(t) \dot{m}_{BLO}(t)$$ (25)

This is a non-linear equation, and on linearization gives,

$$\Delta C_{BLO(t)} \dot{m}_{BLO} + C_{BLO} (\Delta \dot{m}_{BLN}(t))$$ (26)

Substitution for $\Delta \dot{m}_{BLO}(t)$ from Equation (23) results in:

$$\Delta C_{BLO(t)} \dot{m}_{BLO} + C_{BLO} (\Delta \dot{m}_{BLN}(t) - \Delta \dot{M}_{ST} \text{ impressed}(t))$$ (27)

or,

$$\Delta C_{BLO(t)} = \frac{\Delta \dot{m}_{BLN}}{\dot{m}_{BLO}} \Delta C_{BLO(t)}$$.
\[
\frac{(\bar{C}_{BL\ out,\ NBS} - \bar{C}_{BL\ out})}{\bar{M}_{BLO}} \Delta \dot{M}_{BLN}(t) + \frac{\bar{C}_{BLO}}{\bar{M}_{BLO}} \Delta \dot{M}_{ST\ impressed}(t)
\]

Equations (2) and (10) give

\[
\bar{C}_{BL\ out,\ NBS} = \bar{C}_{BL\ out,\ MLB} = \bar{C}_{BLN}
\]

Therefore, Equation (28) can be rewritten as,

\[
\Delta C_{BLO}(t) = \frac{\bar{M}_{BLN}}{\bar{M}_{BLO}} \Delta C_{BL\ out,\ NBS}(t) - \frac{(\bar{C}_{BLO} - \bar{C}_{BLN})}{\bar{M}_{BLN}(t)} \Delta \dot{M}_{BLN}(t)
\]

\[+ \frac{\bar{C}_{BLO}}{\bar{M}_{BLO}} \Delta \dot{M}_{ST\ impressed}(t)\] (30)

The material balance equation for solids entering and leaving an evaporator,

\[
\bar{C}_{WBL} \bar{M}_{WBL} = \bar{C}_{BLO} \bar{M}_{BLO}
\]

can be used to express any of these four variables in terms of the other three. The relation between \(\Delta C_{BL\ out,\ NBS}(t)\) and \(\Delta C_{BLN}\) is given by Equations (8) and (11) as,

\[
\Delta C_{BL\ out,\ NBS} = \frac{e^{-sT_D}}{1 + \tau_6 s} \Delta C_{BLN}
\]

(32)

to dynamically represent the dead time and mixing occurring there, Equation (30) can thus be written as,

\[
\Delta C_{BLO} = \frac{\bar{M}_{BLN}}{\bar{M}_{BLO}} \Delta C_{BLN} - \frac{(\bar{C}_{BLO} - \bar{C}_{BLN})}{\bar{M}_{BLO}} \Delta \dot{M}_{BLN}
\]

\[+ \frac{\bar{C}_{BLO}}{\bar{M}_{BLO}} \Delta \dot{M}_{ST\ impressed}\] (33)
The blocks $G_5$, $G_6$ and $G_7$ in Figure 2 represent the coefficients of $\Delta M_{BLN}$, $\Delta C_{BLN}$, and $\Delta M_{ST}$ impressed respectively in Equation (33).

The heat required to bring the black liquor in each non-boiling section to its boiling temperature depends upon the inlet feed temperature. However, as the latent heat of evaporation is so much greater than the energy required to bring the black liquor to a boil, this derivation of the system equations neglects the variations in the enthalpy of black liquor entering the evaporator. Because of the mixing in the main liquor box, the enthalpy of liquor entering the non-boiling section changes slowly.

Should it be desired to include dynamic, rather than "quasi-steady state" temperature effects, they can be included in the dynamic model by subtracting the output of a first order element fed by the feed temperature, $T_{BLN}$ from the input to block $P_9$ in Figure 2.

The total heat, $Q_{HST}$, transferred from the steam chest goes into heating the black liquor to boiling temperature in the non-boiling section, and to evaporating steam in the boiling section. This can be approximated by:

$$Q_{HST} = M_{BLN} C_{PBLN} (T_{BLO} - T_{BLN}) + \dot{M}_{ST \text{ virt}} \gamma_{BL}$$  

$$= M_{BLN} C_{PBLN} (T_{ST \text{ sat}} + BPR - T_{BLN}) + \dot{M}_{ST \text{ virt}} \gamma_{BL}$$  

where, $T_{ST \text{ sat}}$ is the temperature of saturated vapor at vapor space pressure and, $\dot{M}_{ST \text{ virt}}$ is the mass flow rate of steam generated at a constant vapor space pressure. (Note: the effect of pressure variation on steam flow will be considered later).
\[ T_{ST \ sat} \text{ remains constant at a constant pressure, consequently, Equation (35) can be written for dynamic variations as,} \]

\[ \Delta \dot{Q}_{HST} = \dot{M}_{BLN} C_{PBLN} \Delta BPR + \dot{V}_{BL} \Delta \dot{M}_{ST \ virt} \quad (36) \]

The coefficients of \( \Delta BPR \) and \( \Delta \dot{M}_{ST \ virt} \) are represented by blocks \( P_9 \) and \( P_5 \) respectively in Figure 2.

As the pressure increases or decreases in the vapor space, in addition to a contraction or an expansion of the vapor contained in the boiling section and vapor space of the effect, partial condensation or evaporation of vapor takes place due to absorption or release of heat from the metal tube walls, and boiling black liquor [3]. For a pressure rise in the evaporator, the rate of accumulated heat, \( \dot{Q}_A \), in the black liquor and in the tube walls can be written as:

\[ \dot{Q}_A = M_{BL} C_{PBL} \frac{dT}{dt} + M_M C_{PM} \frac{dT}{dt} \quad (37) \]

where

- \( M_{BL} \) = Mass of black liquor in evaporator
- \( M_M \) = Mass of metal in evaporator
- \( V_V \) = Volume of vapor in boiling and vapor space sections
- \( \rho_V \) = Density of the vapor
- \( C_{PBL} \) = Specific heat of black liquor
- \( C_{PM} \) = Specific heat of metal
- \( T \) = Temperature of metal and black liquor
\( Y_{BL} \) = Heat of evaporation per unit mass of black liquor

The steam production thus diminishes by \( \dot{Q}_A / Y_{BL} \). In addition, the contraction of vapor due to pressure rise will absorb a mass flow rate \( \nu \frac{d \rho_v}{dt} \) from the generated steam. Therefore, the total mass flow rate of steam absorbed, \( \dot{M}_{stored \; BLVS} \), by boiling and vapor space sections can be expressed by:

\[
\dot{M}_{stored \; BLVS} = \left( \frac{M_{BL} C_{PBL} + M_E C_E}{Y_{BL}} \right) \frac{dT}{dt} + \nu \frac{d \rho_v}{dt}
\]

or,

\[
\dot{M}_{stored \; BLVS} = K_{VBTWVS} \frac{dP}{dt}
\]

where,

\[
K_{VBTWVS} = \left( \frac{M_{BL} C_{PBL} + M_E C_E}{Y_{BL}} \right) \frac{dT}{dP} + \nu \frac{d \rho_v}{dP}
\]

Derivatives \( \frac{dT}{dP} \) and \( \frac{d \rho_v}{dP} \) can be evaluated as \( \frac{\Delta T}{\Delta P} \) and \( \frac{d \rho_v}{dP} \) can be evaluated as \( \frac{\Delta T}{\Delta P} = \frac{T_1 - T_2}{P_1 - P_2} \), and \( \frac{\Delta \rho_v}{\Delta P} = \frac{\rho_{V1} - \rho_{V2}}{P_1 - P_2} \) about the saturation temperature corresponding to the operating point vapor pressure in the effect (the effect of super saturation of vapor due to boiling point rise can be neglected as insignificant).

In terms of transformed (Laplace) variables, Equation (40) can be written as,

\[
\dot{M}_{stored \; BLVS} = s K_{VBTWVS} P_{STVPS}
\]
Therefore:

\[ \Delta M_{\text{Stored BLVS}} = s K_{\text{VBLTWVS}} \Delta P_{\text{STVPS}} \]  

(43)

or,

\[ \Delta P_{\text{STVPS}} = \frac{1}{s K_{\text{VBLTWVS}}} \Delta M_{\text{Stored BLVS}} \]  

(44)

This equation is represented by block P6 in Figure 2. Also, the material balance equation for steam can be written as,

\[ \Delta M_{\text{Stored BLVS}} = \dot{M}_{\text{St virt}} - \dot{M}_{\text{ST impressed}} \]  

(45)

where \( \dot{M}_{\text{St virt}} \) and \( \dot{M}_{\text{ST impressed}} \) are the mass flow rate of net steam generated, and the mass flow rate of steam going out of the vapor space respectively.

\( \dot{M}_{\text{ST}} \) is the mass flow rate of steam going from the vapor space of one effect (or from the boiler to the first effect) to the steam chest of a following effect. The pressure drop due to steam flow through the connecting piping is small compared to the upstream pressure. Consequently the steam flow remains subsonic, and the mass flow rate of steam can be expressed by the Darcy Equation [4].

\[ P_{\text{STVPS i}} - P_{\text{STCH i+1}} = C_i \dot{M}_{\text{ST impressed i}}^2 \]  

(46)

\[ C = \frac{f L}{(3600)^2 144 D 2 g A^2 \rho V} \]  

(47)

\( D \) = Internal diameter of pipe in feet

\( f \) = Fanning friction factor

\( L \) = Equivalent length of pipe, in feet

\( P \) = Pressure in psi
\[ g = \text{Acceleration due to gravity (ft/sec}^2) \]
\[ A = \text{Cross-sectional area of pipe} \]
\[ \dot{M}_{\text{ST impressed}} = \text{Mass flow rate of steam (lbs/hr)} \]

Equation (46) reduces on linearization to

\[ \Delta P_{\text{STVPS}} - \Delta P_{\text{HSTCH i+1}} = 2 C_i \dot{M}_{\text{ST impressed i}} \Delta \dot{M}_{\text{ST impressed}} \]  

or,

\[ \Delta \dot{M}_{\text{ST impressed i}} = \frac{\Delta P_{\text{STVPS, i}} - \Delta P_{\text{HSTCH i+1}}}{2 C_i \dot{M}_{\text{ST impressed i}}} \]  

This equation is represented by block P1 in Figure 2.

The dynamical model given in Figure 2 also includes a possibility of a secondary steam being fed to a steam chest. Such a model can also be used for studying those control schemes which may include an additional steam mass flow rate \( \dot{M}_{\text{FSTCH i+1}} \) to steam chest i+1. This secondary steam input may then be used for overcoming a steam deficiency in an effect due to tube fouling. This model can also be used for studying schemes, which may allow bypassing of one effect at a time for cleaning purposes, and are capable of maintaining the desired strong black liquor concentration in the interim period.

The total mass flow rate of steam to the steam chest is then given by,

\[ \dot{M}_{\text{HSTCH i+1}} = \dot{M}_{\text{ST impressed i}} + \dot{M}_{\text{FSTCH i+1}} \]  

For small deviations about the operating point, one can write

\[ \Delta \dot{M}_{\text{HSTCH i+1}} = \Delta \dot{M}_{\text{ST impressed i}} + \Delta \dot{M}_{\text{FSTCH i+1}} \]
SIMPLIFICATION OF THE DYNAMIC MODEL

Two simplifications, one for the connecting pipes between a vapor space and the steam chest and the other for the steam chest of Effect No. 1 can be made in the detailed linear dynamic model given in Figure 2.

The time constant is a fraction of a second for steam flow from the vapor space of one effect to the steam chest of the another. This happens because the resistance to flow of the pipe is very small and thereby the value of gain, \( P_i \), is very large. As a consequence the dynamic pressure difference between a vapor space and the steam chest of the following effect disappears within the same small fraction of a second. The dynamic pressure difference \( \Delta P_{STVPS} - \Delta P_{HSTCH \ i+1} \) can thus be neglected, and the accumulation of steam in the boiling and vapor space sections due to pressure changes in the vapor space of an effect can be combined with the accumulation of steam in the steam chest due to pressure changes in the following effect. The total accumulation of steam, \( \Delta M_{\text{stored}} \), is the sum of the accumulations of steam in the vapor space, the boiling section, and the steam chest. The corresponding equations for accumulation are given by Equations (16) and (43) and thus

\[
\Delta M_{\text{stored}} i = s \left( K_{\text{VBLTWVS} \ i} + K_{\text{VSTCH} \ i+1} \right) \Delta P_{STVPS} \quad (52)
\]

\[
= s K_v \Delta P_{STVPS} \quad (54)
\]

where,

\[
K_v = K_{\text{VBLTWVS} \ i} + K_{\text{VSTCH} \ i+1} \quad (54)
\]
Equation (53), which describes the dynamics of the steam in the boiling and vapor space sections of a particular Effect \(i\) and in steam chest of the next Effect \((i+1)\), is represented by block \(D_6\) in Figure 3. Block \(D_6\) replaces blocks \(P_6\), \(P_1\), and \(P_2\) in Figure 2.

The time constant for a steam chest alone is only about 2 seconds, and therefore the dynamics of steam storage in the steam chest of Effect 1 can be ignored. It may be noted that as far as the dynamics is concerned, the steam chests in other effects behave as part of the previous effects, and therefore should not be automatically ignored. The time constant of the differential equation for the steam dynamics in the steam chest for Effect 1, is about 1.4 seconds and its dynamics have been replaced by an algebraic equation.

Both the above simplifications are given in Figure 3.
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SECTION VI
MATHEMATICAL MODELING OF THE RECOVERY UNIT

INTRODUCTION

A mathematical process model serves at least two useful purposes in the design of a control system. Primarily it is a concise description of all relevant information about the process. Secondly, as one very rarely has access to a process for extensive experimentation, the testing of control schemes may be done by simulation of the mathematical model on a computer together with the corresponding model of the proposed control system.

The model has been developed for the C.E. recovery unit at Valdosta. Except for different parameter values the model will be valid for similar furnaces with different capacities. Parts of the model will have to be modified for the Babcock & Wilcox type recovery unit. These parts are the drying of the liquor spray, the combustion air system, and the direct contact evaporator.

For the purposes of this present study the recovery unit was broken down into smaller units for analysis purposes. This makes the model more manageable and more flexible than it would have been if it were designed as one large unit. Figure 1 shows the components into which the recovery unit has been subdivided.

Most of the divisions are along boundaries of physical equipment, and need no further comment. A few boundaries require some explanation:
FIGURE 1
SUBDIVISION OF RECOVERY UNIT MODEL
1. The primary zone extends from the char bed surface to the beginning of the secondary air ports.

2. The secondary zone extends from the primary zone to the screen tubes.

3. The superheater zone is the region from the secondary zone to midway between the end of the last superheater tube bank and the beginning of the boiler tube bank.

4. The boiler zone extends from the superheater zone to midway between the end of the boiler tube bank and the beginning of the economizer tube bank.

5. The economizer zone extends from the boiler zone to the cascade evaporator inlet.

The sequence of unit modeling used was that of actual material flow in the process. Equations were based mainly on material and energy balances, and in some cases were supplemented by empirical functions where exact models could not be formulated. A complete glossary of the variables used is given at the end of this Section. The energy balance was taken relative to a reference temperature of 80°F.

In order to simplify the notations, the superscript is omitted for all variables and parameters that belong to the particular furnace subsection in question. For example, in the Section on black liquor heaters the superscript (h) will be omitted, but superscripts on variables from other furnace sections are retained. A key to the notations is given in the glossary.
The black liquor has been divided into the following components (with the weight fraction of each component in the liquor shown in parenthesis):

1. Input solids, \( X_{\text{bls}} \). These are the total solids from the dissolved wood and the digester chemicals. The black liquor from the multiple-effect evaporators normally contain only input solids and water.

2. Salt cake, \( X_{\text{Na}_2\text{SO}_4} \). This is sodium sulfate which is added to the liquor in the precipitator (as recovered particulates), the cascade evaporator (as recovered particulates and ash), and the salt cake mixing tank (as makeup chemicals).

3. Carbonate, \( X_{\text{Na}_2\text{CO}_3} \). This is sodium carbonate which is added to the liquor in the precipitator (as recovered particulates), and in the cascade evaporator (as recovered particulates and ash).

4. Water, \( X_{\text{blw}} \). Water is removed in the cascade evaporator, and some is added in the black liquor heaters.

The sum of the weight fractions of the black liquor must equal unity.

\[
X_{\text{bls}} + X_{\text{Na}_2\text{SO}_4} + X_{\text{Na}_2\text{CO}_3} + X_{\text{blw}} = 1
\]  

The input solids have been decomposed into the following components (with the weight fraction of each component in the solids shown in parenthesis):
1. Hydrogen, \( x_{H}^{(bl)} \).

2. Sodium Sulfide, \( x_{Na_2S}^{(bl)} \). This component is separated out because it is responsible for the generation of hydrogen sulfide \( H_2S \) in the cascade evaporator.

3. Oxygen, \( x_{O_2}^{(bl)} \).

4. Carbon, \( x_{C}^{(bl)} \).

5. Sodium not as sodium sulfide, \( x_{Na}^{(bl)} \).

6. Sulfur not as sodium sulfide, \( x_{S}^{(bl)} \).

The sum of the weight fractions of the input solids must equal unity.

\[
X_H^{(bl)} + X_{Na_2S}^{(bl)} + X_O^{(bl)} + X_C^{(bl)} + X_{Na}^{(bl)} + X_S^{(bl)} = 1 \quad (2)
\]

Elements other than the above will occur in small quantities only and can be neglected in the material balance.
BLACK LIQUOR HEATERS

Two direct contact black liquor heaters are used to raise the temperature of the black liquor from the outlet temperature of the cascade evaporator to the required spray temperature.

Heating is accomplished by injecting steam into the liquor. The temperature response is immediate for the present modeling purpose and a slight dilution of the black liquor results due to the condensed steam.

The temperature increase caused by the first heater does not enter the model directly. Thus the two heaters will be included in one, giving the total temperature increase.

The equations describing the material and energy balances for the heater are: (The superscript (h) on $w^h_{bl}$, $w^h_{st}$, $T^h_{bl}$, $H^h_{st}$, $T^h_{st}$, and the $X_i$ has been omitted.)

MATERIAL BALANCE

Total flow

$$w^h_{bl} = w^h_{bl} + w^h_{st}$$  (3)

Water

$$w^h_{bl} X^h_{blw} = w^h_{bl} X^h_{blw} + w^h_{st}$$  (4)

Input solids

$$w^h_{bl} X^h_{bls} = w^h_{bl} X^h_{bls}$$  (5)
Salt cake

\[ \omega_{bl} X_{Na_2SO_4} = \omega_{bl} X_{(ce)} X_{(ce)} \]  

(6)

Carbonate

\[ X_{Na_2CO_3} = 1 - X_{blw} - X_{bls} - X_{Na_2SO_4} \]  

(7)

ENERGY BALANCE

Liquor temperature

\[
T_{bl} = \frac{1}{\omega_{bl} [X_{blw} c_{pw} + (1-X_{blw})c_{pbls}]} \left[ \omega_{bl} \left( X_{(ce)} c_{pw} + (1-X_{(ce)})c_{pbls} \right) \left( T_{(ce)} - 80 \right) + \omega_{st} \left( H_{st} + c_{pw} (T_{st} - 80) \right) \right] + 80
\]  

(8)

\( T_{st} \) is the saturation temperature for the heater steam, and \( H_{st} \) is the heat of vaporization at temperature \( T_{st} \). The specific heat of black liquor input solids, \( c_{pbls} \), is used for the total content of solids in the liquor. The energy equation is made algebraic because the dynamics are too fast to be of any significance.

In the simulation of the black liquor heater, the temperature controller will be included as a part of the heater. Instead of using the steam flow \( \omega_{st} \) as input variable, the heater set point temperature \( T_{bl} \) will be used. The dynamics are neglected.
Solving Equation (8) for \( w_{st} \) yields

\[
w_{st} = \frac{1}{H_{st} + c_{pw}(T_{st} - T_{bl})} \left[ w_{bl}^{(ce)} \left( x_{blw} c_{pw} + (1 - x_{blw}) c_{pb1s} \right) (T_{bl} - T_{bl}^{(ce)}) \right] \tag{9}
\]

where the reference temperature has been set equal to \( T_{bl} \) in order to reduce the number of terms.

**SPRAY NOZZLES**

The black liquor from the last heater goes to a set of spray nozzles located in openings in the furnace walls located approximately 13 ft above the bottom of the furnace. The nozzles may have internal plates for rotating the liquor as it leaves, but the plates can also be removed. The nozzle can then be considered a pressure nozzle. Removal of the plates makes the flow less sensitive to disturbances caused by lumps of solids in the liquor.

The spray pattern from a nozzle can be characterized by a droplet distribution function, that is, the fraction of the total volume flow due to droplets with a diameter less or equal to a given number as a function of that number. This distribution function is a function of nozzle geometry and size, and of such liquor properties as nozzle pressure, liquor solids concentration and liquor temperature.

Unfortunately there are no good mathematical models available in the literature that relate the above variables to a spray distribution function.
Marshall [19] presents a number of semiempirical expressions but none for black liquor sprays. He concludes that so far no theoretically developed expression seems to satisfy all experimental data, and that one should choose the best empirical representation obtainable in each case to represent the particular droplet distribution at hand.

Kennedy [20] states that the liquor should have a viscosity of about 125 centipoises for spraying, and 250 centipoises for pumping. He presents a chart showing the absolute viscosity as a function of temperature and solids concentration, Figure 2. The viscosity appears to be very sensitive with respect to solids concentration, and less sensitive with respect to liquor temperature.

From actual furnace operational experience one learns, however, that the drop-size distribution is very sensitive with regard to the liquor temperature from the last black liquor heater. A temperature change of 4-6°F can change a coarse spray to a fine mist. The black liquor heaters both increase the water content and raise the temperature of the liquor at the same time. The variations in total solids content and total temperature are slight, however, and it seems doubtful that the strong effect on the drop-size distribution can be explained fully by Figure 2.

An experiment performed by Mr. Frode Galtung in the Valdosta recovery furnace related the sensitivity of the spray distribution to variations in the total solids content in the
FIGURE 2

ABSOLUTE VISCOSITY OF SULFATE WASTE LIQUOR

(From [20])
black liquor. Normal operation required a salt cake addition of 2400 lb/hr. This was reduced to zero for a period of 30 minutes, and the effect on the spray pattern was visually observed. No change was visible, although the change in total solids concentration was from 65% to 63.8%. According to Figure 2, this change in solids concentration would be equivalent to a temperature change of approximately 15°F. It may therefore be concluded that either the salt cake affects the viscosity of the black liquor to a much lesser extent than the original black liquor solids from the digester, or that a secondary effect of black liquor temperature other than the viscosity change is present.

Hochmuth [21] explains the drying process from the spray as one of partial flashing of the liquor's water content. The spray temperature is kept above the atmospheric boiling point of the liquor. When the liquor is released from the spray nozzles, the flashed water will have the action of expanding the initial spray particles to many times their original size. The increased particle surface will then cause further rapid evaporation.

This effect will add to the effect of temperature on viscosity, and may explain why the drop-size distribution is so sensitive with respect to the final liquor temperature.

Due to the uncertainties with regard to the exact mechanism that forms the drop-size distribution and to the lack of data on the actual distribution it was decided to
use a very simple model. The drop-size distribution used is presented as a function of liquor temperature in Figure 3. Only three regions are of interest in the present model:

1. The volume fraction of the spray due to droplets of diameter 10 μm or less. This is assumed to account for the fine sodium particulates that go to the precipitator and are partially recovered there. They will always be entrained by the furnace gases.

2. The volume fraction of the spray due to droplets of diameter 500 μm or more. These are too large to be entrained by the gases, even when the furnace is operating under maximum load.

3. The intermediate volume fraction of droplets in the diameter range 10-500 μm. The amount of entrainment is determined by the velocity of the upward moving gases in the primary zone.

Thus only three parameters are being used in the definition of the drop-size distribution:

- $T_{b11}$ is the temperature below which all droplets are larger than 500 μm. No fraction of the spray will be entrained at this temperature.

- $T_{b12}$ is the temperature above which all droplets are less than 10 μm. All of the liquor will be entrained at this temperature.
FIGURE 3
DROP-SIZE DISTRIBUTION FUNCTION
- $T_{bl3}$ is the temperature above which all droplets are less than 500 μm. More or less of the liquor may be entrained at this temperature, depending on the gas velocities in the primary zone.

The equations describing the drop-size distribution are: (The superscript (sp) has been omitted on the $T_i$.)

**Fraction of spray equal to or smaller than 10 μm**

$$Y_2 = \frac{T_{bl1} - T_{bl1}}{T_{bl2} - T_{bl1}} \quad T_{bl1} \leq T_{bl1} \leq T_{bl2} \quad (10)$$

**Fraction of spray equal to or larger than 500 μm**

$$Y_1 = \begin{cases} \frac{T_{bl3} - T_{bl1}}{T_{bl3} - T_{bl1}} & T_{bl1} \leq T_{bl1} \leq T_{bl3} \\ 0 & T_{bl3} \leq T_{bl1} \leq T_{bl2} \end{cases} \quad (11)$$

The composition of the liquor from the spray nozzles is the same as that from the black liquor heaters.

**Entrainment.**

Depending on the drop-size distribution from the spray nozzles, a certain fraction of the flow will be entrained by the upward moving gases in the primary zone. The gases are due to primary air, infiltration air, combustible gases released from the char bed, and water evaporating from the char bed surface. All droplets below a certain size are assumed to be entrained.
Fraction of spray going to char bed

\[
1 - n_1 = Y_1 \frac{u_g}{u_{g1}} + (1 - Y_2) \left( 1 - \frac{u_g}{u_{g1}} \right)
\]  

where \( n_1 \) is the volume fraction of the black liquor flow which is entrained by the gases. As the liquor is assumed to be homogeneous the volume fraction will be identical to the weight fraction. \( u_g \) is the vertical velocity of the gases in the primary zone. \( u_{g1} \) is the vertical gas velocity at maximum load on the furnace.

When \( u_g = u_{g1} \), then \( Y_1 \) is the fraction going to the char bed. This corresponds to the fraction of the spray due to droplets equal to or larger than 500 \( \mu \)m. When \( u_g \) is very small, then \( 1 - Y_2 \) is the fraction going to the char bed. This corresponds to the fraction of the spray due to droplets larger than 10 \( \mu \)m. The fraction \( Y_2 \) due to droplets equal to or smaller than 10 \( \mu \)m is always assumed to be entrained.

The gas velocity can be written

\[
u_g = \frac{w_g}{\rho_g A_f}
\]

where \( w_g \) is the total vertical gas flow in the primary zone. \( \rho_g \) is the average density of the gas flow. \( A_f \) is the furnace crosssectional area.

The total vertical gas flow is

\[
w_g = w_a + w_{ia} + w_0^{(cm)} + w_H^{(cm)} + w_C^{(cm)} + w_w^{(cs)}
\]
The first two terms are the primary air and the primary infiltration air. The next three terms are the gases released from the burning char bed, and the last term is the water from the spray being vaporized on the char bed surface.

The water \( w^{(cs)}_w \) that goes to the char bed with the black liquor, and subsequently evaporates will be a function of the entrainment \( \eta_1 \). The last term of (14) must therefore be eliminated.

The water flow to the char bed can be written in terms of the entrainment ratio

\[
\frac{w^{(cs)}_w}{w_{bl}} = \frac{w^{(sp)}_{bl}}{N^{(sp)}_{bl}} x^{(sp)}_{blw} (1 - \eta_1) \quad (15)
\]

where \( w^{(sp)}_{bl} \) is the liquor flow through one spray nozzle, \( N^{(sp)}_{bl} \) is the number of spray nozzles, and \( x^{(sp)}_{blw} \) is the weight fraction of water in the liquor through the spray nozzles.

From (12) and (15)

\[
\frac{w^{(cs)}_w}{w_{bl}} = \frac{w^{(sp)}_{bl}}{N^{(sp)}_{bl}} x^{(sp)}_{blw} \left[ Y_1 \frac{u_g}{u_{g1}} + (1 - Y_2) \left[ 1 - \frac{u_g}{u_{g1}} \right] \right] \quad (16)
\]

Substituting (13) and (16) into (14) and solving for \( u_g \) yields

\[
u_g = \frac{w^{(1)}_a + w^{(1)}_{ia} + w^{(cm)}_g + w^{(sp)}_{bl} \frac{N^{(sp)}_{bl}}{x^{(sp)}_{blw}} (1 - Y_2)}{\rho_g A_f \left[ 1 + \frac{w^{(sp)}_{bl}}{\rho_g A_f u_{g1}} \frac{N^{(sp)}_{bl}}{x^{(sp)}_{blw}} (1 - Y_1 - Y_2) \right]} \quad (17)
\]
where
\[ w_g^{(cm)} = w_0^{(cm)} + w_H^{(cm)} + w_C^{(cm)} \] (18)

The model does not account for any evaporation to the gas stream from the liquor droplets that are large enough to reach the char bed surface. The reason for this is that little data have been found on the evaporation rate from black liquor droplets under actual furnace conditions. If data were available then evaporation can easily be included in the model. It is likely that the rate of water flow to the char bed surface has a strong controlling effect on the combustion rate. As the evaporation rate will increase with increasing spray surface, and hence with increasing liquor temperature the net effect of a liquor temperature change on the corresponding change in water flow to the char bed surface will be larger than that due to the change in entrainment alone.

The assumption made in the present model is that the change in entrainment due to liquor temperature variations accounts for the major change in water flow to the char bed surface.

The model also neglects any pyrolysis or combustion of droplets in suspension in the primary zone. The water in the entrained droplets is assumed to evaporate in the primary zone, while the combustion takes place in the secondary zone.
Equations for the entrained black liquor are: (The superscript \((pe)\) on \(w_{bl}\) and the \(X_i\) has been omitted.)

**MATERIAL BALANCE**

Total flow

\[
w_{bl} = w_{bl} = w_{bl} N_{(sp)} \eta_1 \quad (19)
\]

Total hydrogen

\[
X_H = X_{bls} X_{(blce)} + X_{blw} \left( \frac{2M_H}{M_{H_2O}} \right) \quad (20)
\]

Total oxygen

\[
X_O = X_{bls} X_{(blce)} + X_{blw} \left( \frac{M_O}{M_{H_2O}} \right) + X_{sp} \left( \frac{4M_O}{M_{Na_2SO_4}} \right)

+ X_{Na_2CO_3} \left( \frac{3M_O}{M_{Na_2CO_3}} \right) \quad (21)
\]

Total sulfur

\[
X_S = X_{bls} \left[ X_{(blce)} + X_{Na_2S} \left( \frac{M_S}{M_{Na_2S}} \right) \right] + X_{sp} \left( \frac{M_S}{M_{Na_2SO_4}} \right) \quad (22)
\]

Total carbon

\[
X_C = X_{bls} X_{(blce)} + X_{Na_2CO_3} \left( \frac{M_C}{M_{Na_2CO_3}} \right) \quad (23)
\]

Total sodium

\[
X_{Na} = 1 - X_H - X_O - X_S - X_C \quad (24)
\]
The composition of both the entrained liquor and the part going to the char bed surface is the same as that of the liquor coming from the spray nozzles.

The liquor that is not entrained is assumed to reach the char bed surface: (The superscript (spc) on the $w_i$ has been omitted.)

Total liquor flow to char bed

$$w_{bl} = w_{bl}^{(sp)} N_{(sp)} - w_{bl}^{(pe)}$$

(25)

Net flow of input solids

$$w_{bls} = w_{bl} X_{bls}$$

(26)

Net flow of salt cake

$$w_{Na_2SO_4} = w_{bl} X_{Na_2SO_4}^{(sp)}$$

(27)

Net flow of carbonate

$$w_{Na_2CO_3} = w_{bl} X_{Na_2CO_3}^{(sp)}$$

(28)

Total solids flow

$$w_{blts} = w_{bls} + w_{Na_2SO_4} + w_{Na_2CO_3}$$

(29)

Components of total solids flow

Hydrogen

$$w_H = w_{bls} X_{H}^{(blce)}$$

(30)
Carbon not as carbonate

\[ w_C = w_{\text{bls}} \times (\text{blce}) \]

(31)

Carbon as carbonate

\[ w_{\text{C}}(\text{Na}_2\text{CO}_3) = w_{\text{Na}_2\text{CO}_3} \left( \frac{M_C}{M_{\text{Na}_2\text{CO}_3}} \right) \]

(32)

Sulfur not as salt cake

\[ w_S = w_{\text{bls}} \left[ X_{S}^{(\text{blce})} + X_{\text{Na}_2S}^{(\text{blce})} \left( \frac{M_S}{M_{\text{Na}_2S}} \right) \right] \]

(33)

Sulfur as salt cake

\[ w_{S}(\text{Na}_2\text{SO}_4) = w_{\text{Na}_2\text{SO}_4} \left( \frac{M_S}{M_{\text{Na}_2\text{SO}_4}} \right) \]

(34)

Sodium

\[ w_{\text{Na}} = w_{\text{bls}} \left[ X_{\text{Na}}^{(\text{blce})} + X_{\text{Na}_2S}^{(\text{blce})} \left( \frac{2M_{\text{Na}}}{M_{\text{Na}_2S}} \right) \right] \]

\[ + w_{\text{Na}_2\text{SO}_4} \left( \frac{2M_{\text{Na}}}{M_{\text{Na}_2\text{SO}_4}} \right) + w_{\text{Na}_2\text{CO}_3} \left( \frac{2M_{\text{Na}}}{M_{\text{Na}_2\text{CO}_3}} \right) \]

(35)

Oxygen

\[ w_O = w_{\text{blts}} - w_H - w_C - w_{\text{C}}(\text{Na}_2\text{CO}_3) - w_S \]

\[ - w_{S}(\text{Na}_2\text{SO}_4) - w_{\text{Na}} \]

(36)
CHAR BED

The following main assumptions have been made:

1. Water in the liquor reaching the char bed surface evaporates instantaneously.

2. All sodium and sulfur in the solids reaching the char bed surface remain in the char bed or leave with the smelt.

3. The char bed is assumed to be homogeneous (perfectly mixed) for material balance purposes.

4. The rate of reaction of char bed solids (conversion of char bed solids into smelt and combustible gases) is proportional to the product of the mass fraction of carbon (not as carbonate) and an Arrhenius term. The temperature in the Arrhenius term is the average temperature of the char bed surface layer.

5. The reduction efficiency of the smelt is determined by the model of Bauer and Dorland [11].

6. The oxygen deficiency in the Bauer and Dorland model is taken equal to the average theoretical oxygen deficiency above the char bed surface in the primary zone.

7. The temperature in the Bauer and Dorland model is taken equal to the surface layer temperature of the char-bed.

8. The surface layer temperature is determined by taking an energy balance for the total char bed, using a pseudo volume to match the temperature dynamics.
9. The bulk density of the char bed is assumed constant. The following equations have been developed for the energy and material balance of the char bed: (The superscript (cb) on $\rho$, $V$, $V_p$, $H_2O$, $\dot{Q}$, $A$, $U_r$, $C_p$, $C_{pg}$, and the $X_i$ has been omitted.)

**MATERIAL BALANCE**

Evaporation of water

$$w_{(cs)}^{(spc)} = w_{(bl1)}^{(spc)} X_{blw}$$  \(37\)

Char Bed Composition

**Total mass**

$$\frac{d}{dt} (\rho V) = w_{(blts)}^{(spc)} - w_{(cm)}$$  \(38\)

where $w_{(spc)}^{(blts)}$ is the net flow of solids to the char bed surface and $w_{(cm)}$ is the net flow of solids from the char bed surface due to the generation of smelt and combustibles. As the bulk density is assumed constant the equation for the char bed volume becomes

$$\frac{d}{dt} V = \frac{1}{\rho} \left( w_{(spc)}^{(blts)} - w_{(cm)} \right)$$  \(39\)

**Rate of reaction**

$$w_{(cm)} = K_{cm} X_C \cdot \exp \left[ - \frac{\alpha_C}{T_C + 460} \right]$$  \(40\)

The reaction rate is proportional to the fraction of carbon (not as carbonate) and an Arrhenius term involving the char bed surface layer temperature $T_C$. 

Carbon not as carbonate

\[
\frac{d}{dt}(\rho \, V \, X_C) = w(C) - w(cm) \, X_C
\]  \hspace{1cm} (41)

which combined with (2.39) yields

\[
\frac{d}{dt} \, X_C = \frac{1}{\rho \, V} \left[ w(spc) - w(spc) \, X_C \right]
\]  \hspace{1cm} (42)

Similarly we get for the other components of the char bed

Carbon as carbonate

\[
\frac{d}{dt} \, X_C(Na_2CO_3) = \frac{1}{\rho \, V} \left[ w(spc) - w(spc) \, X_C(Na_2CO_3) \right]
\]  \hspace{1cm} (43)

Sodium

\[
\frac{d}{dt} \, X_{Na} = \frac{1}{\rho \, V} \left[ w(spc) - w(spc) \, X_{Na} \right]
\]  \hspace{1cm} (44)

Hydrogen

\[
\frac{d}{dt} \, X_H = \frac{1}{\rho \, V} \left[ w(spc) - w(spc) \, X_H \right]
\]  \hspace{1cm} (45)

Sulfur not as salt cake

\[
\frac{d}{dt} \, X_S = \frac{1}{\rho \, V} \left[ w(spc) - w(spc) \, X_S \right]
\]  \hspace{1cm} (46)

Sulfur as salt cake

\[
\frac{d}{dt} \, X_S(Na_2SO_4) = \frac{1}{\rho \, V} \left[ w(spc) - w(spc) \, X_S(Na_2SO_4) \right]
\]  \hspace{1cm} (47)

Oxygen

\[
X_O = 1 - X_C - X_H - X_S - X_{Na} - X_C(Na_2CO_3)
- X_S(Na_2SO_4)
\]  \hspace{1cm} (48)
Input solids

\[ X_{\text{bls}} = 1 - X_S(\text{Na}_2\text{SO}_4) \left( \frac{M_{\text{Na}_2\text{SO}_4}}{M_S} \right) - X_C(\text{Na}_2\text{CO}_3) \left( \frac{M_{\text{Na}_2\text{CO}_3}}{M_C} \right) \]  

(49)

Carbon for combustion from reacting char

\[ w_C^{(cm)} = w_{(cm)} (X_C + X_C(\text{Na}_2\text{CO}_3)) - \frac{w_{(sm)} X_{(sm)} X_C}{50} \]  

(50)

The first term represents the total carbon "released" due to the reaction while the second term is the amount of carbon going out of the furnace as smelt.

Hydrogen for combustion from reacting char

\[ w_H^{(cm)} = w_{(cm)} X_H \]  

(51)

All the hydrogen from the black liquor solids is released for combustion.

Oxygen for combustion from reacting char

\[ w_O^{(cm)} = w_{(cm)} - \frac{w_{(sm)} X_S}{52} - w_C^{(cm)} - w_H^{(cm)} \]  

(52)

Smelt composition (as elements)

Sodium

\[ \frac{w_{(sm)} X_{(sm)} X_{Na}}{53} = w_{(cm)} X_{Na} \]  

(53)

Sulfur

\[ \frac{w_{(sm)} X_S X_{(sm)} X_{S(\text{Na}_2\text{SO}_4)}}{54} = w_{(cm)} (X_S + X_S(\text{Na}_2\text{SO}_4)) \]  

(54)
Carbon

\[ w_{cm} X_{sm} = w_{cm} \cdot \frac{1}{2} \left[ X_{Na} \cdot 2 \left( X_S + X_S(\text{Na}_2\text{SO}_4) \right) \left( \frac{M_{Na}}{M_S} \right) \right] \left( \frac{M_C}{M_{Na}} \right) \] (55)

Oxygen

\[ w_{sm} X_{O(sm)} = w_{sm} \cdot 4 \left( 1 - \eta_r \right) \left[ X_S + X_S(\text{Na}_2\text{SO}_4) \right] \left( \frac{M_O}{M_S} \right) + 3 \left( w_{cm} X_{C(sm)} \right) \left( \frac{M_O}{M_C} \right) \] (56)

Total flow of smelt

\[ w_{sm} = w_{sm} X_{Na} + w_{sm} X_S + w_{sm} X_C + w_{sm} X_O \] (57)

Reduction ratio

\[ \eta_r = \frac{\# \text{ moles Na}_2\text{S}}{\# \text{ moles Na}_2\text{S} + \# \text{ moles Na}_2\text{SO}_4} \]

\[ = \frac{X_{Na} X_{sm} \text{M} \text{Na}_2\text{SO}_4}{X_{Na} X_{sm} \text{M} \text{Na}_2\text{SO}_4 + X_{Na} X_{sm} \text{M} \text{Na}_2\text{S}} \] (58)

It is assumed that \( \eta_r \) can be expressed according to Figure 4 which is taken from the article by Bauer and Dorland [11]. The temperature is taken as that of the char bed surface, \( T_c \). The oxygen deficiency, \( -\Delta \) is taken as the average oxygen deficiency in the primary zone. This is computed with the same formula as that used to compute excess oxygen in the combustion gases from the recovery furnace.
FIGURE 4
REDUCTION EFFICIENCY DIAGRAM
(From [11])
Smelt Composition (As Chemicals)

Sodium sulfide

\[
X_{\text{Na}_2\text{S}} = \frac{w_{\text{cm}}}{w_{\text{sm}}} \left( X_S + X_S(\text{Na}_2\text{SO}_4) \right) \eta_1 \left( \frac{M_{\text{Na}_2\text{S}}}{M_S} \right) \quad (59)
\]

Salt cake

\[
X_{\text{Na}_2\text{SO}_4} = \frac{w_{\text{cm}}}{w_{\text{sm}}} \left( X_S + X_S(\text{Na}_2\text{SO}_4) \right) \left( 1 - \eta_1 \right) \left( \frac{M_{\text{Na}_2\text{SO}_4}}{M_S} \right) \quad (60)
\]

Carbonate

\[
X_{\text{Na}_2\text{CO}_3} = 1 - X_{\text{Na}_2\text{S}} - X_{\text{Na}_2\text{SO}_4} \quad (61)
\]

Required oxygen flow for complete combustion of gases given off by char bed reaction

\[
w_{\text{O}}(1t) = w_{\text{H}}(\text{cm}) \left( \frac{M_O}{2M_H} \right) + w_{\text{C}}(\text{cm}) \left( \frac{2M_O}{M_C} \right) \quad (62)
\]

Flow of available oxygen from primary (and infiltration) air

\[
w_{\text{O}}(1) = \left( w_{\text{a}}(1) + w_{\text{ia}}(1) \right) X_{\text{a}1} \quad (63)
\]

Combustion air availability in primary zone

\[
F(1) = \frac{w_{\text{O}}(1)}{w_{\text{O}}(1t) - w_{\text{O}}(\text{cm})} \quad (64)
\]

Oxygen concentration in the primary zone

\[
\Delta = \frac{100 \cdot (F(1) - 1)c_{O_2}}{X_g(1) + 100 \cdot (F(1) - 1)} \quad (65)
\]
Equation (65) can be used to compute the concentration of oxygen in the combustion gases from a recovery furnace. The numerator is the percentage of air excess (or deficiency), multiplied by the oxygen concentration in the combustion air, \( c_{O_2} \). The denominator is the total amount of combustion products. \( K_1 \) is a parameter that must be adjusted to the particular "excess air-oxygen concentration curve" for the recovery furnace. This is done in Appendix A. \( \Delta \) is computed as Vol \% \( O_2 \). Oxygen deficiency is indicated when \( \Delta < 0 \).

**ENERGY BALANCE**

Combustion energy of reacting char

\[
\dot{Q}_t^{(c)} = w^{(cm)} \left[ X_{b_{bls}} H_{b_{bls}} - X_{S} H_{S} - X_{H_{2}O} \left( \frac{M_{H_{2}O}}{2M_{H}} \right) \right] \quad (66)
\]

The total available heat of combustion of the black liquor solids is computed as the calorimetric heat value \( H_{b_{bls}} \) corrected for reduction of sulfur and formation of water, all at 80°F.

Combustion energy released in primary zone and char bed

\[
\dot{Q}_t^{(c_1)} = \dot{Q}_t^{(c)} \left( \frac{w_0^{(1)} + w_0^{(cm)}}{w_0^{(1_t)}} \right) \quad (67)
\]

It is assumed that all available oxygen in the primary zone plus that given off from the char bed release combustion energy on a proportional basis. Normally a primary zone oxygen deficiency exists, and hence a part of \( \dot{Q}_t^{(c)} \) will be released in the secondary zone.
Combustion energy released in the char bed

\[ \dot{Q} = \dot{Q}^{(c1)} \eta^{(c)} \] (68)

\(\eta^{(c)}\) represents the fraction of the combustion energy released in the char bed and the primary zone which actually is released in the char bed due to combustion of solid char.

Combustion energy released above the char bed in the primary zone

\[ \dot{Q}^{(1)} = \dot{Q}^{(c1)} - \dot{Q} \] (69)

\(\dot{Q}^{(1)}\) is the energy released by burning gases that have been formed from the reacting char.

Radiant heat to water walls from char bed surface

\[ \dot{Q}_b = A U_r ((T_c + 460)^4 - (T_b + 460)^4) \] (70)

A is the area of the char bed surface, \(U_r\) is the radiant heat transfer coefficient, \(T_c\) is the char bed temperature, and \(T_b\) is the boiler water temperature. The surface of the water wall tubes are for the purpose of heat transfer assumed to have the same temperature as the water in the boiler [16, pp. 6-5, 6-6].
Char bed energy balance

\[
\frac{d}{dt}(\rho \ V \ c_p \ T_c) = \dot{Q} + w_{bl}^{(spc)} \left[x_{blw}^{(spc)} \ c_{pw} + (1-x_{blw}^{(spc)})c_{plws}\right] \\
(T_{bl}^{(sp)} - 80) - w_{bl}^{(spc)} x_{blw}^{(spc)} \left[c_{pwv} (T_{bl}^{(sp)} - 80) + H_{H2O}\right] \\
- \dot{Q}_b - w_{sm}^{(cm)} \left[c_p (T_{sm} - 80) + H_{sm}^{(cm)}\right] \\
- (w_{cm}^{(cm)} - w_{sm}^{(cm)}) c_{pg} (T_c - 80) - w_{cm}^{(cm)} x_S (Na_2SO_4) H_{S^{nT}}
\]

The terms on the right are the energy of combustion in the char bed, the energy of the liquor in the spray, the energy required to evaporate the water in the spray (it is assumed that the steam from the char bed surface has the liquor temperature \(T_{bl}^{(sp)}\)), the radiant energy to the water walls, the energy content of the leaving smelt (the smelt temperature \(T_{sm}\) will be assumed constant), the energy content of the combustibles from the reacting char bed solids and the energy required to reduce the salt cake in the black liquor (this is not included in the computation of \(\dot{Q}_t^{(c)}\)). Heat transfer between the burning gases in the primary and secondary zone and the char bed surface other than that which can be accounted for by the distribution of the combustion energy release is neglected. The model of the energy balance is rather crude, but necessarily so due to the lack of data concerning the chemical and thermodynamic reactions in this part of the furnace.
Char bed temperature

\[
\frac{dT_c}{dt} = \frac{1}{\rho \, V_p \, c_p} \left[ Q + w_{bl} (spc) (1 - X_{blw} (spc)) c_{pb1s} (T_{bl} - 80) \\
+ w_{bl} (spc) X_{blw} (spc) \left[ (c_{pw} - c_{pwv}) (T_{sp} - 80) - H_{H_2O} \right] \\
- \dot{Q}_b - w_{sm} (cm) \left[ c_p (T_{sm} - 80) + H_{sm} \right] \\
- (w_{sm} (cm) - w_{sm} (cm)) c_{pg} (T_c - 80) - w_{sm} (cm) \alpha (Na_2SO_4) H_{ss} \eta_r \right]
\]

The char bed volume \( V \) has been replaced by a constant volume \( V_p \). \( V_p \) is a smaller pseudovolume which represents the surface layer of the char bed. The surface temperature of the char bed is assumed to control the rate of reaction, Equation (40), and it will have a faster dynamics than that of the whole char bed. \( V_p \) is used as a parameter to match the char bed surface temperature dynamics to that of a real furnace.

**PRIMARY ZONE**

All the water in the entrained portion of the spray is assumed to evaporate in the primary zone, but no combustion of the entrained spray takes place.

The equations for the energy and material balance are:

(The superscript (1) on \( w_g, w_a, w_{ia}, \rho_g, V_g, c_{pg}, T_g, c_{pa}, \)
\( T_a, T_{ia}, \dot{Q} \) and the superscript (gl) on \( \dot{Q}_b, A_b, U_r, \) and the \( X_i \) have been omitted)
MATERIAL BALANCE

All solids and gases are split up into their elementary components.

Hydrogen

\[ w_g X_H = (w_a + w_{ia}) X_H^{(a1)} + w_{cm} + w_{bl} w_{blw} \left( \frac{2M_H}{M_{H_2O}} \right) + w_{bl} (pe) X_{(blce)} \]

The terms are the hydrogen from the water vapor in the primary air and the primary zone infiltration air, from the reacting char, from the total water content of the liquor from the spray nozzles (includes both the water from the entrained spray and the evaporation from the char bed surface), and from the black liquor solids in the entrained spray.

Oxygen

\[ w_g X_O = (w_a + w_{ia}) X_O^{(a1)} + w_{cm} + w_{bl} N(sp) X_{(sp)} \left( \frac{M_O}{M_{H_2O}} \right) \]

\[ + w_{bl} \left[ X_{bls} X_{(blce)} + X_{Na_2SO_4} \left( \frac{4M_O}{M_{Na_2SO_4}} \right) + X_{Na_2CO_3} \left( \frac{3M_O}{M_{Na_2CO_3}} \right) \right] \]

Sulfur

\[ w_g X_S = w_{bl} X_{bls} \left( \frac{M_S}{M_{Na_2SO_4}} \right) \]

\[ + X_{Na_2SO_4} \left( \frac{M_S}{M_{Na_2SO_4}} \right) \]
Sulfur is provided from the solids in the entrained liquor only. This is one of the more uncertain assumptions, as the path of sulfur in the recovery furnace is not yet established. There may be a certain amount of sulfur escaping from the char bed surface, but due to the lack of data, this is ignored.

Carbon

\[ w_g X_C = w_C \left[ X_{bl} + X_{bl} \right] + \left[ X_{sp} X_{bl} \right] + \left[ X_{sp} \right] \left( \frac{M_C}{M_{Na_2CO_3}} \right) \]  

(76)

Carbon from the primary air is negligible.

Sodium

\[ w_g X_{Na} = w_{bl} X_{Na} \]  

(77)

As for sulfur it is assumed that all the sodium comes from the entrained solids in the spray. There may also in this case be some sodium escaping from the char bed surface due to sublimation, but this is neglected.

Nitrogen

\[ w_g X_N = (w_a + w_{ia}) X_{N} \]  

(78)

Nitrogen from the black liquor solids is negligible.

Total flow to secondary zone

\[ w_g = w_g X_H + w_g X_O + w_g X_S + w_g X_C + w_g X_{Na} + w_g X_N \]  

(79)
ENERGY BALANCE

Radiant heat to water walls from the hot gases

\[ \dot{Q}_b = A_b U_r \left( (T_g + 460)^4 - (T_b + 460)^4 \right) \]  \hspace{1cm} (80)

\( A_b \) is the area of the furnace walls in the primary zone, \( U_r \) is the radiant heat transfer coefficient, \( T_g \) is the gas temperature, and \( T_b \) is the temperature of the water in the boiler.

Gas energy balance

\[ \frac{d}{dt}(\rho V g c_p g T_g) = w_a c_{pa}(T_a - 80) + w_{ia} c_{pa}(T_{ia} - 80) \]

\[ + w_{bl} \left[ c_{pbl} (T_{bl} - 80) - \frac{T_{blw}}{H_2O} \right] \]

\[ + w_{cw} c_{pwv}(T_{cw} - 80) + (w_{cm} c_{cm})(cb)(T_c - 80) \]

\[ + \dot{Q} - \dot{Q}_b - w g c_{pg}(T_g - 80) \]  \hspace{1cm} (81)

The first two terms are the heat contents of the primary- and primary infiltration air. The following terms are the heat content and the heat of vaporization (at 80°F) of the black liquor entrained, the heat content of water vapor from the char bed surface, the heat content of combustible gases from the char bed, the primary zone heat of combustion, the radiant heat transferred to the furnace walls, and the heat content of the gases going to the secondary zone.
Equation (81) can be made algebraic in order to eliminate the relatively fast dynamics of the gas temperature. In this case an iterative solution of the radiant heat transfer term is required in order to get a usable expression for $T_g$.

Equation (2.80) can be written

$$\dot{Q}_b = A_b \left( T_g - T_b \right)$$

$$U_{rl} = U_r \frac{(T_g + 460)^4 - (T_b + 460)^4}{T_g - T_b} \quad (82)$$

Gas temperature

$$T_g = \frac{1}{A_b U_{rl} + w_g c_{pg}} \left[ w_{pa} c_{pa} (T_a - 80) + w_{ia} c_{pa} (T_{ia} - 80) + w_{bl} (c_{pbl} (T_{b1} - 80) - X_{blw} H_{2O}) + w_{sw} (c_{pwh} (T_{b1} - 80) + (w_{cm} - w_{sm}) c_{pg} (T_c - 80) + \dot{Q} + A_b U_{rl} (T_b - 80) \right] + 80 \quad (84)$$

SECONDARY ZONE

The main assumptions that have been made are the following:

1. The conditions in the secondary zone determine the final composition of the combustion gases and the particulates.
2. The formation of $\text{SO}_2$, $\text{H}_2\text{S}$ and $\text{CO}$ is determined mainly by the amount of excess oxygen and the degree of turbulence from the injection of secondary combustion air. Empirical relationships based on data from Thoen et al. [4] have been used. The sulfur for the formation of $\text{SO}_2$ and $\text{H}_2\text{S}$ is subtracted from the total sulfur available before any other sulfurous compounds are formed.

3. If sufficient sulfur is available after the formation of $\text{H}_2\text{S}$ and $\text{SO}_2$, then all the sodium in the entrained fine droplets ($\leq 10 \mu\text{m}$) will form salt cake. If sufficient sulfur is not present, then the rest of the sodium will form sodium carbonate. The products from the fine droplets will be called particulates.

4. The sodium in the entrained large droplets ($> 10 \mu\text{m}$) will form salt cake with whatever sulfur is left from the reaction of the small droplets. The rest of the sodium forms carbonate. The products from the large droplets will be called fly ash.

5. The carbon available after the previous steps will form carbon dioxide.

6. The hydrogen present will form water.

7. The nitrogen will pass unchanged.

8. The oxygen left over will be in the form of $\text{O}_2$.

Equations for the material and energy balance of the secondary zone are: (The superscript (2) on $w_g$, $\rho_a$, $v_a$, $w_a$, $A_{po}$, $w_{ia}$, $\dot{\rho}_g$, $T_g$, $\rho_g$, $V_g$, $c_{pg}$, $c_{pa}$, $T_a$, $T_{ia}$, and the...
superscript (g2) on $K_{SO_2}$, $K_{H_2S}$, $K_{CO}$, $\dot{Q}_b$, $A_b$, $U_r$, $U_r^2$, and the $X_i$ have been omitted.}

MATERIAL BALANCE

Sulfur dioxide

$$w_g X_{SO_2} = K_{SO_2} w_g^{(1)} X_S^{(g1)} \cdot \exp\left[ -\alpha_{SO_2} \delta - \beta_{SO_2} X_{O_2}^{(dg2)} \right]$$  \hspace{1cm} (85)

The formation rate of $SO_2$ is assumed to be proportional to the sulfur flow to the secondary zone, and exponentially dependent on the degree of turbulence from the injection of secondary air $\delta$, and the fraction of oxygen as $O_2$ in dry gas in the secondary zone, $X_{O_2}^{(dg2)}$. $K_{SO_2}$, $\alpha_{SO_2}$ and $\beta_{SO_2}$ are the parameters.

Hydrogen sulfide

$$w_g X_{H_2S} = K_{H_2S} w_g^{(1)} X_S^{(g1)} \cdot \exp\left[ -\alpha_{H_2S} \delta - \beta_{SO_2} X_{O_2}^{(dg2)} \right]$$  \hspace{1cm} (86)

Carbon monoxide

$$w_g X_{CO} = K_{CO} w_g^{(1)} X_C^{(g1)} \cdot \exp\left[ -\alpha_{CO} \delta - \beta_{CO} X_{O_2}^{(dg2)} \right]$$  \hspace{1cm} (87)

The formation rate of $CO$ is proportional to the carbon flow to the secondary zone.

Turbulence function

$$\delta = \rho_a (v_a)^2$$  \hspace{1cm} (88)

$\delta$ represents the kinetic energy per unit volume of secondary air injected into the furnace. The secondary air is injected
tangentially into the upward moving combustion gases in order to give as good turbulence effect as possible. \( \rho_a \) and \( v_a \) are the secondary air density and the air velocity through the secondary air ports respectively, (\( v_a \) has dimensions ft/sec).

The mass flow of secondary air

\[
\dot{w}_a = v_a A_{po} \rho_a \cdot 3,600 \quad (89)
\]

\( A_{po} \) is the total area of the secondary air ports

Substitution of (89) into (88) yields:

\[
\delta = \frac{1}{\rho_a} \left( \frac{\dot{w}_a}{A_{po} \cdot 3,600} \right)^2 \quad (90)
\]

A sulfur sufficiency condition is used to determine if there is enough sulfur to form salt cake of all the sodium in the fine droplets from the entrained liquor spray.

Sulfur sufficiency condition

\[
\dot{w}_{bl1}(sp)N_{(sp)}Y_z X_{(blc)} \left( \frac{M_S}{2M_{Na}} \right) + X_{(blc)} \left( \frac{M_S}{M_{Na_2S}} \right) + X_{Na_2SO_4} \left( \frac{M_S}{M_{Na_2SO_4}} \right) + X_{Na_2CO_3} \left( \frac{M_S}{M_{Na_2CO_3}} \right)
\]

\[
\leq \dot{w}_{bl1}(sp)X_{(g1)} - \dot{w}_g \left( \frac{M_S}{M_{SO_2}} \right) - \dot{w}_g \left( \frac{M_S}{M_{H_2S}} \right) \quad (91)
\]
Salt cake particulates

If sufficient sulfur

\[ w_{gX}Na_2SO_4p = w_{bl}X_{Na_2SO_4} + X_{Na_2S} + X_{Na_2CO_3} \]  \hspace{1cm} (92)

If insufficient sulfur

\[ w_{gX}Na_2So_4p = \left[ w_{gX}(g) - w_{gXSO_2} \right] - w_{gXH_2S} \]  \hspace{1cm} (93)

Carbonate particulates

If sufficient sulfur

\[ w_{gX}Na_2CO_3p = 0 \]  \hspace{1cm} (94)

If insufficient sulfur

\[ w_{gX}Na_2CO_3p = \left[ w_{b1}(sp) \right] 2M_{Na} \left( \frac{Na_2SO_4}{Na_2CO_3} \right) \]  \hspace{1cm} (95)
Salt cake fly ash
If sufficient sulfur

\[ w_{g}X_{Na_{2}SO_{4}fa} = w_{g}(1)x(g_{1}) \left( \frac{M_{Na_{2}SO_{4}}}{MS} \right) - w_{g}X_{Na_{2}SO_{4}p} \]
\[ - w_{g}XSO_{2} \left( \frac{M_{Na_{2}SO_{4}}}{MSO_{2}} \right) - w_{g}XH_{2}S \left( \frac{M_{Na_{2}SO_{4}}}{M_{H_{2}S}} \right) \]  \hspace{1cm} (96)

If insufficient sulfur

\[ w_{g}X_{Na_{2}SO_{4}fa} = 0 \] \hspace{1cm} (97)

Carbonate fly ash

\[ w_{g}X_{Na_{2}CO_{3}fa} = \left[ w_{g}(1)x(g_{1}) - \left( w_{g}X_{Na_{2}SO_{4}p} + w_{g}X_{Na_{2}SO_{4}fa} \right) \right] \cdot \left( \frac{2M_{Na}}{M_{Na_{2}SO_{4}}} \right) - w_{g}X_{Na_{2}CO_{3}p} \left( \frac{2M_{Na}}{M_{Na_{2}CO_{3}}} \right) \left( \frac{M_{Na_{2}CO_{3}}}{2M_{Na}} \right) \] \hspace{1cm} (98)

Carbon dioxide

\[ w_{g}X_{CO_{2}} = \left[ w_{g}(1)x(g_{1}) - w_{g}X_{CO} \left( \frac{M_{C}}{M_{CO}} \right) - \right. \left. w_{g}X_{Na_{2}CO_{3}p} \right] \cdot \left( M_{CO} \right) \left( \frac{M_{CO_{2}}}{M_{C}} \right) + w_{g}X_{Na_{2}CO_{3}fa} \left( \frac{M_{CO_{2}}}{M_{Na_{2}CO_{3}}} \right) \] \hspace{1cm} (99)

Water

\[ w_{g}X_{H_{2}O} = \left[ w_{g}(1)x(g_{1}) + (w_{a} + w_{ia})x(a_{2}) \right] \cdot \left( \frac{2M_{H}}{M_{H_{2}O}} \right) \left( \frac{M_{H_{2}O}}{2M_{H}} \right) - w_{g}X_{H_{2}S} \left( \frac{M_{H_{2}O}}{M_{H_{2}S}} \right) \left( \frac{M_{H_{2}O}}{2M_{H}} \right) \] \hspace{1cm} (100)
Nitrogen

\[ w_g X_{N_2} = w_g^{(1)} X_N^{(1)} + (w_a + w_{ia}) X_N^{(a_2)} \]  \hspace{1cm} (101)

Oxygen

\[ w_g X_{O_2} = w_g^{(1)} + w_a + w_{ia} - w_g X_{Na_2SO_4} \]
\[ - w_g X_{Na_2CO_3} - w_g X_{Na_2SO_4} - w_g X_{Na_2CO_3} \]
\[ - w_g X_{SO_2} - w_g X_{H_2S} - w_g X_{CO} - w_g X_{CO_2} \]
\[ - w_g X_{H_2O} - w_g X_{N_2} \]  \hspace{1cm} (102)

It is assumed that there will be some oxygen left to form oxygen gas.

Total flow to superheater zone

\[ w_g = w_g^{(1)} + w_a + w_{ia} \]  \hspace{1cm} (103)

Weight fraction of oxygen in dry gas

\[ X_{O_2}^{(dg)} = \frac{w_g X_{O_2}}{w_g (1 - X_{H_2O} - X_{Na_2CO_3} - X_{Na_2SO_4} - X_{Na_2CO_3} - X_{Na_2SO_4} - X_{Na_2SO_4} - X_{Na_2CO_3})} \]  \hspace{1cm} (104)
ENERGY BALANCE

Combustion energy released in secondary zone

\[ \dot{Q}_g = \dot{Q}_t(c) - \dot{Q}_t(c_1) + w_{bl} X_{bls} \left[ H_{bls} - X_H H_{2O} \left( \frac{M_{H_2O}}{2M_H} \right) \right] \]

\[ - w_g X_{CO} H_{CO} - w_g X_{H_2S} H_{2S} \]

(105)

On the right hand side of the equation are the total combustion energy available from the reacting char, the part of the total combustion energy which is released in the char bed and the primary zone, the total available combustion energy of the entrained black liquor solids (corrected for the formation of water), the loss of combustion energy due to the formation of CO, and the loss of combustion energy due to the formation of H_2S. The energy loss due to the formation of SO_2 has not been considered.

Radiant heat to water walls from the hot gases

\[ \dot{Q}_b = A_b U_r \left( (T_g + 460)^a - (T_b + 460)^a \right) \]

(106)

A_b is the area of the furnace walls in the secondary zone, U_r is the radiant heat transfer coefficient, T_g is the gas temperature, and T_b is the temperature of the water in the boiler.

Gas energy balance

\[ \frac{d}{dt} \left( \rho_g V_g c_{pg} T_g \right) = \dot{Q}_g + w_{g} c_{pg} (T_g - 80) + w_a c_{pa} (T_a - 80) \]

\[ + w_{ia} c_{pa} (T_{ia} - 80) - \dot{Q}_b - w_g c_{pg} (T_g - 80) \]

(107)
The combustion energy release, the heat content of the gases from the primary zone, the heat content of the secondary combustion air and the secondary infiltration air, the heat transferred to the furnace walls, and the heat content of the gases going to the superheater zone, make up the right hand side of the equation.

Equation (107) can be made algebraic in order to eliminate the relatively fast dynamics of the gas temperature. In this case an iterative solution of the radiant heat transfer term is required in order to get a usable expression for $T_g$.

Equation (106) can be written:

$$\dot{Q}_b = A_b \ U_{rl} \ (T_g - T_b) \quad (108)$$

$$U_{rl} = U_r \ \frac{(T_g + 460)^4 - (T_b + 460)^4}{T_g - T_b} \quad (109)$$

Gas temperature

$$T_g = \frac{1}{A_b \ U_{rl} + \ \ \ w_g \ c_{pg}} \ \left[ \dot{Q}_g + \ \ \ w^{(1)}_g c^{(1)} \ (T^{(1)}_g - 80) \right.$$

$$\left. + \ \ w_a \ c_{pa} (T_a - 80) + \ \ w_{ia} \ c_{pa} (T_{ia} - 80) + A_b \ U_{rl} \ (T_b - 80) \right]$$

$$+ \ 80 \quad (110)$$
SUPERHEATER ZONE

In the superheater zone heat is transferred to the furnace wall and screen tubes by radiation, \( \dot{Q}_b \), and to the superheater tube bank by convection, \( \dot{Q}_{\text{sh}} \). The main assumptions that have been made are:

1. The steam temperature in the superheater is constant. This is not a necessary assumption for the modeling purpose, but it simplifies the model and can be justified by the present use of desuperheater water in an automatic steam temperature control system. The assumption is only valid as long as the heat transfer rate to the superheater is large enough to allow a flow of desuperheater water. This is usually the case during normal operation of the furnace.

2. The dynamics of the gas and superheater tube temperatures are relatively fast and are neglected.

3. The steam from the superheater is released to a high pressure header by a constant pressure valve. The steam pressure in the superheater can therefore be considered constant. A pressure drop between the boiler drum and the superheater outlet is caused by the steam flow through the superheater. This pressure drop is actually a function of the steam flow rate but will be assumed constant for the purpose of model simplification. A consequence of this assumption is that the drum pressure and water temperature in the boiler are constant.
4. Soot blowing is normally practiced on a regular basis according to experience on the rate of deposits formation. In the model the effect of soot blowing on the heat transfer coefficient has been neglected due to the lack of data.

Equations for the energy and material balance of the superheater zone are: (The superscript (3) on $w_g$, $w_{sb}$, $w_{st}$, $w_{dw}$, $T_g$, $c_{pg}$, $T_{st}$, $H_{st}$, $T_{st}$, and the superscript (g3) on $Q_b$, $A_b$, $U_r$, $U_r'$, $U_c$, $Q_{sh}$, and the $X_i$ are omitted.)

MATERIAL BALANCE

Water in combustion gas

$$w_g \cdot H_2O = w_g^{(2)} \cdot H_2O + w_{sb} \quad (111)$$

The flow of water in the combustion gases to the boiler zone equals the flow of water from the secondary zone plus the steam used for soot blowing in the superheater zone.

Total flow of combustion gas

$$w_g = w_g^{(2)} + w_{sb} \quad (112)$$

For the rest of the gases and particulates

$$w_g \cdot X_i = w_g^{(2)} \cdot X_i \quad (113)$$

Steam flow from superheater

$$w_{st} = w_{st}^{(s)} + w_{dw} - w_{sbt} \quad (114)$$
The steam flow out of the superheater equals the sum of the steam flow from the boiler and the flow of desuperheater water minus the flow of steam for soot blowing.

Total steam flow for soot blowing

\[ w_{sbt} = w_{sb} + w_{s(b)} + w_{sb}^{(s)} \]  \hspace{1cm} (115)

Soot blowers are used in the superheater, boiler, and economizer.

ENERGY BALANCE

Radiant heat to water walls and screen tubes from the hot gases

\[ \dot{Q}_b = A_b \ U_r \ (T_g + 460)^4 - (T_b + 460)^4 \]  \hspace{1cm} (116)

The equation can be written

\[ \dot{Q}_b = A_b \ U_r \ (T_g - T_b) \]  \hspace{1cm} (117)

\[ U_{r(g)} = U_r \ \frac{(T_g + 460)^4 - (T_b + 460)^4}{T_g - T_b} \]  \hspace{1cm} (118)

Gas temperature

\[ T_g = \frac{A_b \ U_{r(g)} + U_c \ A_{sh} + w_g \ c_{pg} \ \left[ w_g^{(2)} \ c_g^{(2)} \ (T_g^{(2)} - 80) \right.}{w_{sb} \ H_{sb} + 80} + A_b \ U_{r(g)} (T_b - 80) + A_{sh} \ U_c \ (T_{st} - 80) \]  \hspace{1cm} (119)

The solution for \( T_g \) is found by iteration on Equations (118) and (119).
The entries in the brackets are the heat content of the gases from the secondary zone, heat transfer to the furnace water walls, heat transfer to the steam in the superheater tubes, and the heat content of the soot blowing steam (relative to 80°F). An overall convective heat transfer term is used to represent the heat transfer between the combustion gases and the superheated steam.

Because the superheated steam enthalpy $H_{st}$ is assumed constant, the flow of desuperheater water can be computed once the steam flow $w_{st}^{(u)}$ from the boiler is given.

Desuperheater water flow

$$w_{dw} = \frac{1}{H_{st} - H_{w}^{(u)}} \left[ Q_{sh} - w_{st}^{(u)} \left( H_{st} - H_{st}^{(u)} \right) \right]$$  \hspace{1cm} (120)

$$Q_{sh} = A_{sh} U_c (T_g - T_{st})$$  \hspace{1cm} (121)

$Q_{sh}$ is the rate of heat transfer from the combustion gases to the superheater tubes. In (2.120) the difference between $Q_{sh}$ and the heat required to heat the steam flow, $w_{st}^{(u)}$, from the boiler must be accounted for by evaporation and heating of desuperheater water.

**BOILER ZONE**

In the boiler zone heat is transferred from the combustion gases to the boiler tube bank. Water from the boiler is bled off as continuous blow down.

The main assumptions are:
1. The temperature of the water and steam in the boiler tubes is constant and equal to the saturation temperature of water at the constant boiler pressure.

2. The boiler level and feedwater control system works perfectly so that boiler water dynamics can be neglected.

3. The boiler gas temperature dynamics is neglected.

4. The total furnace heat loss is constant.

Equations for the energy and material balance for the boiler zone are: (The superscript \(4\) on \(w_g, w_{sb}, T_g, c_{pg}, w_{st}, H_{st}, w_{bd}, H_w\), and the superscript \(g4\) on \(\dot{Q}_b, A_b, U_c\), and the \(X_i\) have been omitted.)

**Material Balance**

Water vapor in the combustion gas

\[
 w_g X_{H_2O} = w_g^{(s)} X_{H_2O}^{(s)} + w_{sb} \tag{122}
\]

The flow of water vapor in the combustion gases to the economizer zone equals the flow of water vapor from the superheater zone plus the steam used for soot blowing in the boiler.

Total flow of combustion gas

\[
 w_g = w_g^{(s)} + w_{sb} \tag{123}
\]

For the rest of the gases and particulates the equations are the same as \((113)\).
ENERGY BALANCE

Heat flow to the boiler bank from the gas

\[ \dot{Q}_b = A_b \cdot U_c \cdot (T_g - T_b) \]  \hspace{1cm} (124)

The boiler temperature \( T_b \) is assumed to be constant.

Total heat flow to the boiler water

\[ \dot{Q}_{bt} = \dot{Q}_b + \dot{Q}_{b(g^3)} + \dot{Q}_{b(g^2)} + \dot{Q}_{b(g^1)} + \dot{Q}_{b(cb)} \]  \hspace{1cm} (125)

The total heat flow is the sum of the energy flows transferred to boiler water in all parts of the furnace.

Gas temperature

\[ T_g = \frac{1}{A_b U_c + \frac{w_g}{c_p} \cdot \frac{w_g}{c_p} \cdot \frac{c_p}{c_p}} \left[ \frac{w_{(s)}}{c_p} \cdot \left( T_{g(5)} - 80 \right) + A_b \cdot U_c \cdot (T_b - 80) \right] 
+ \frac{w_{sb} \cdot H_{sb}}{c_p} + 80 \]  \hspace{1cm} (126)

The heat content of the gases from the superheater zone, heat transfer to the boiler bank, and the heat content of the soot blowing steam make up the contents of the brackets.

Steam production

\[ w_{st} = \frac{1}{H_{st} - H_w} \left[ \dot{Q}_{bt} - \dot{Q}_{g} - \left( w_{bd} + w_{dw} \right) \left( H_w - H_w^{(s)} \right) \right] \]  \hspace{1cm} (127)

The terms are the total energy flow to the boiler water, the total furnace heat loss, and the energy taken out of the boiler by the continuous blow down and the flow of desuperheater water. The enthalpy of both the blow down and the
desuperheater water are assumed equal to the enthalpy of the boiler water, \( H_w \). The enthalpy of the steam from the boiler is \( H_{st} \).

Equations (128) and (120) can be solved explicitly for \( w_{st} \) and \( w_{dW}^{(s)} \).

The result for \( w_{st} \) is

\[
\dot{Q}_{bt} - \dot{Q}_l - w_{bd}\left(H_w - H_{w}^{(s)}\right) - \dot{Q}_{sh} \frac{H_w - H_{w}^{(s)}}{H_{st} - H_w} \]

\[
w_{st} = \frac{H_{st} - H_{w}^{(s)} - \frac{\left(H_{w} - H_{st}\right) \left(H_w - H_{w}^{(s)}\right)}{H_{st} - H_w}}{(128)}
\]

**ECONOMIZER ZONE**

In the economizer zone heat is transferred from the combustion gases to the economizer tube bank.

The main assumptions are:

1. The gas temperature dynamics are neglected.
2. The temperature of the economizer tubes is equal to the economizer water temperature [16, pp. 6-5 to 6-6].
3. The economizer has been lumped and is described by one water temperature.

Equations for the energy and material balances of the economizer zone are: (The superscript (5) on \( w_g, w_{sb}, w_w, \dot{Q}_{ec}, T_g, T_w, c_{pg}, c_{pw}, H_{wi}, T_{wi}, H_w, m_{ec}, c_{pec}, m_{w}, \) and the superscript (g5) on \( A_{ec}, U_c, A_{ecmx}, \) and the \( X_i \) have been omitted.)
MATERIAL BALANCE

Water in combustion gas

\[ w_g X_{H_2O} = w_g X(g^4) + w_{sb} \]  \hspace{1cm} (129)

The flow of water in the combustion gases to the cascade evaporator equals the flow of water from the boiler zone plus the steam used for soot blowing in the economizer.

Total flow of combustion gas

\[ w_g = w_g^{(4)} + w_{sb} \]  \hspace{1cm} (130)

For the rest of the gases and particulates the equations are the same as (2.113).

Flow of water through economizer

\[ w_w = w_{st}^{(4)} + w_{bd}^{(4)} + w_{dw}^{(3)} \]  \hspace{1cm} (131)

The flow through the economizer equals the water evaporated in the boiler, the flow of continuous blow down, and the flow of desuperheater water.

ENERGY BALANCE

Heat flow to economizer tube bank from the gas

\[ Q_{ec} = A_{ec} U_c (T_g - T_w) \]  \hspace{1cm} (132)

\( T_w \) is the temperature of the water in the economizer.
Exposed area of economizer

\[ A_{ec} = A_{ecmx} \eta_{ec} \quad (133) \]

\( A_{ecmx} \) is the maximum effective economizer area. \( \eta_{ec} \) represents the effect of the economizer bypass dampers. The bypass dampers shield parts of the heat transfer surfaces from exposure to the hot gases. They are used to control the gas temperature of the gases going to the cascade evaporator. Only small temperature variations can be obtained in this manner.

\[ 0 < \eta_{ecmn} \leq \eta_{ec} \leq 1 \quad (134) \]

\( \eta_{ecmn} \) is the minimum value that \( \eta_{ec} \) can attain. Only a certain amount of the heat transfer surface can be shielded away.

Gas temperature

\[ T_g = \frac{1}{A_{ec} U_c + w_g c_p g} \left[ w_g^{(u)} c_p^{(u)} (T_g^{(u)} - 80) + A_{ec} U_c (T_w - 80) \right. \]
\[ + w_{sb} H_{sb} \bigg] + 80 \quad (135) \]

where the energy contributions are from the heat content of the gases from the boiler zone, heat transfer to the economizer, and the heat content of the soot blowing steam.
Economizer water temperature

\[
\frac{dT_w}{dt} = \frac{1}{m_{ec} c_{pec} + m_w c_{pw}} \left[ Q_{ec} + w_w H_{wi} \right.
\]

\[
- w_w \left[ H_{wi} + c_{pw} (T_w - T_{wi}) \right] \right]
\] (136)

The terms on the right are the heat transfer to the economizer, the heat content of the water entering the economizer, and the heat content of the water leaving the economizer for the boiler.

Enthalpy of water to boiler

\[
H_w = H_{wi} + c_{pw} (T_w - T_{wi})
\] (137)

T_{wi} is the temperature of the water entering the economizer.

**CASCADE EVAPORATOR AND SALT CAKE ADDITION**

The combustion gases from the economizer are directed through the cascade evaporator where they pick up moisture from the liquor on the cascade evaporator wheel. Almost all of the heat given off by the gases is converted into heat of evaporation of water and heating of the water vapor, [10, pp. 625]. The black liquor enters the vat from the precipitator and leaves for the salt cake mixing tank after evaporation. The wheel rotates with constant speed. The motor current is recorded and used as a measure for the concentration of solids in the vat liquor. The liquor level is usually kept constant although it is controlled by
a level control system. If the black liquor contains sodium sulfide (usually the case if black liquor oxidation is not used) then hydrogen sulfide will be formed according to the reaction (Thoen [4]):

\[
\text{CO}_2 + \text{Na}_2\text{S} + \text{H}_2\text{O} + \text{H}_2\text{S} + \text{Na}_2\text{CO}_3
\]

Mercaptans can also be formed but will not be considered here. A certain amount of the sulfur dioxide in the gas from the economizer may be absorbed in the cascade evaporator. This effect will be ignored in the model, however. Weak black liquor can be added to the liquor in the vat for dilution purposes if the vat liquor concentration becomes too high.

The main assumptions are:

1. The gas temperature dynamics are neglected.
2. Water evaporates from the liquor on the surface of the wheel only, not from the vat. The rate of evaporation is proportional to the temperature difference between the cascade evaporator gas and wheel surface temperature.
3. The wheel surface temperature is assumed to be at the boiling temperature of black liquor at an average solids concentration for the liquor in the vat. The wheel temperature therefore is kept constant.
4. All of the salt cake and carbonate fly ash is precipitated in the cascade evaporator. These larger ash particles will be caught by the wet surface of the
wheel or they will hit the liquor in the vat directly. The contents of the ash hopper that collects ash falling off the boiler tubes is also normally emptied into the vat.

5. None of the salt cake and carbonate particulates are precipitated in the cascade evaporator but are passed on to the precipitator. This is not strictly true, but serves as a useful simplification since little data on the amounts of particulates collected in the cascade evaporator are available.

6. The salt cake addition is assumed to take place in the cascade evaporator vat. This simplification reduces the number of equations required.

7. The rate of generation of hydrogen sulfide is according to the chemical reaction on page 84 proportional to the concentration of both Na$_2$S and CO$_2$ in the black liquor. In the computation of the reaction rate it is assumed that the concentration of CO$_2$ in the reacting liquor is proportional to the weight fraction of CO$_2$ in the combustion gases entering the cascade evaporator from the economizer zone. The concentration of Na$_2$S is assumed proportional to the weight fraction of Na$_2$S in the black liquor.

8. The composition of the input solids in the weak dilution liquor is equal to the composition of input solids in the strong liquor entering the vat.
9. The liquor in the vat is perfectly mixed.

Equations for the energy and material balance of the cascade evaporator are: (The superscript (ce) on $w_g$, $R_H^2S$, $R_{H_2O}$, $A_{wh}$, $K_{H_2O}$, $T_g$, $T_{wh}$, $K_{H_2S}$, $\rho_{bl}$, $V_{bl}$, $w_{sc}$, $w_{bl}$, $w_{bld}$, $\rho_{bld}$, $\rho_{H_2O}$, $c_{pg}$, $U_{wh}$, $A_V$, $U_V$, $T_{bl}$, $c_{pfa}$, $c_{psl}$, $c_{pbl}$, $T_{bld}$, $T_{sc}$, $H_{H_2O}$, and the $X_i$ has been omitted.)

MATERIAL BALANCE FOR GAS

Sulfur dioxide

\[ w_g X_{SO_2} = w_g (s) x(g)_{SO_2} \]  \hspace{1cm} (138)

Hydrogen sulfide

\[ w_g X_{H_2S} = w_g (s) x(g)_{H_2S} + R_{H_2S} \]  \hspace{1cm} (139)

$R_{H_2S}$ is the formation rate of $H_2S$ in the cascade evaporator.

Carbon monoxide

\[ w_g X_{CO} = w_g (s) x(g)_{CO} \]  \hspace{1cm} (140)

Carbon dioxide

\[ w_g X_{CO_2} = w_g (s) x(g)_{CO_2} - R_{H_2S} \left( \frac{M_{CO_2}}{M_{H_2S}} \right) \]  \hspace{1cm} (141)

Water

\[ w_g X_{H_2O} = w_g (s) x(g)_{H_2O} + R_{H_2O} \]  \hspace{1cm} (142)

$R_{H_2O}$ is the evaporation rate of water.
Nitrogen
\[ w_g X_{N_2} = w^{(s)}_g X_{N_2} \] (143)

Oxygen
\[ w_g X_{O_2} = w^{(s)}_g X_{O_2} \] (144)

Salt cake particulates
\[ w_g X_{Na_2SO_4p} = w^{(s)}_g X_{Na_2SO_4p} \] (145)

Carbonate particulates
\[ w_g X_{Na_2CO_3p} = w^{(s)}_g X_{Na_2CO_3p} \] (146)

Total flow of gas and particulates
\[ w_g = w_g^{(s)} + R_{H_2S} \left(1 - \frac{M_{CO_2}}{M_{H_2S}}\right) + R_{H_2O} \\
- w_g^{(s)} \left[ X_{Na_2SO_4fa} + X_{Na_2CO_3fa} \right] \] (147)

where the total flow of gas, particulates, and fly ash from the economizer zone, the net mass exchange due to the formation of \( H_2S \), the evaporation of water and the loss of the fly ash to the liquor in the vat represent the contributions to the total gas material balance.

Evaporation rate
\[ R_{H_2O} = A_{wh} K_{H_2O} (T_g - T_{wh}) \] (148)
A_{wh} is the total wheel evaporation surface, \( K_{H_2O} \) is the mass transfer coefficient, \( T_g \) is the gas temperature, and \( T_{wh} \) is the wheel surface temperature. \( T_{wh} \) is assumed to be constant.

Formation rate of hydrogen sulfide

\[
R_{H_2S} = A_{wh} K_{H_2S} X_{bls} X_{(blce)} X_{Na_2S} X_{(gs)} \tag{149}
\]

\( K_{H_2S} \) is a formation rate coefficient. \( X_{bls}, X_{(blce)}, X_{(gs)} \) are the weight fractions of input solids in the vat liquor, sodium sulfide in the input solids, and carbon dioxide in the gas from the economizer, respectively.

MATERIAL BALANCE FOR THE BLACK LIQUOR IN THE VAT

Salt cake

\[
\frac{d}{dt} (\rho_{bl} V_{bl} X_{Na_2SO_4}) = w_{(pr)} X_{(pr)} + w_{(s)} X_{Na_2SO_4,fa} + w_{sc} - w_{bl} X_{Na_2SO_4} \tag{150}
\]

where the flow of salt cake in the liquor from the precipitator, the salt cake fly ash from the economizer gas, the salt cake added as makeup chemical, and the salt cake leaving with the liquor from the vat are included.

Vat liquor total mass

\[
\frac{d}{dt} (\rho_{bl} V_{bl}) = w_{(pr)} + w_{bl} d + w_{(s)} \left[ X_{Na_2SO_4,fa} + X_{Na_2CO_3,fa} \right] - R_{H_2O} + w_{sc} + R_{H_2S} \left[ \frac{M_{CO_2}}{M_{H_2S}} - 1 \right] - w_{bl} \tag{151}
\]
The terms are the liquor flow from the precipitator, the flow of dilution liquor, the fly ash from the gas, the evaporation of water, the addition of salt cake makeup, the formation of hydrogen sulfide, and the liquor leaving the vat.

Total liquor flow from vat

As the vat volume $V_{bl}$ is constant, the volumetric flow of liquor from the vat is equal to the volumetric flow of liquor to the vat, - if we neglect the shrinking effect of mixing liquors of different composition.

$$\frac{w_{bl}}{\rho_{bl}} = \frac{w_{(pr)}}{\rho_{(pr)}} + \frac{w_{bl}}{\rho_{bl}} - \frac{R_{H2O}}{\rho_{H2O}}$$ \hspace{1cm} (152)

The total volume flow is equal to the volume flow from the precipitator plus the volume flow for dilution minus the change in volume flow due to evaporation. $\rho_{H2O}$ will be used as a parameter to adjust the equation to the operating data. The mass flow of liquor is then

$$w_{bl} = \frac{\rho_{bl}}{\rho_{(pr)}} w_{(pr)} + \frac{\rho_{bl}}{\rho_{bl}} w_{bl} - \frac{\rho_{bl}}{\rho_{H2O}} R_{H2O}$$ \hspace{1cm} (153)

Expansion of the left side of (2.150) yields

$$\frac{d}{dt} (\rho_{bl} V_{bl} X_{Na2SO4}) = V_{bl} \left[ \rho_{bl} \frac{d}{dt} X_{Na2SO4} + X_{Na2SO4} \frac{d}{dt} \rho_{bl} \right]$$ \hspace{1cm} (154)
By substitution of (154), (151) and (153) into (150) the equation becomes for the fraction of salt cake in the vat liquor

\[
\frac{d}{dt} x_{Na_2SO_4} = \frac{1}{V_{bl} \rho_{bl}} \left[ w_{bl} \rho_{bl} \left( x_{(pr)} \left( x_{Na_2SO_4} - x_{Na_2SO_4} \right) - \left[ w_{g} x_{Na_2CO_3 fa} + w_{bl} - R_{H_2O} + R_{H_2S} \left( \frac{M_{CO_2}}{M_{H_2S}} - 1 \right) \right] x_{Na_2SO_4} + \left[ w_{sc} + w_{g} x_{Na_2SO_4 fa} \left( 1 - x_{Na_2SO_4} \right) \right] \right) \right]
\]

Equation (153) into (151) gives for the vat liquor density

\[
\frac{d}{dt} \rho_{bl} = \frac{1}{V_{bl} \rho_{bl}} \left[ w_{bl} \rho_{bl} \left( 1 - \rho_{bl} \rho_{(pr)} \right) + w_{bl} \left( 1 - \frac{\rho_{bl}}{\rho_{bl} + \rho_{H_2O}} \right) - R_{H_2O} \left( 1 - \frac{\rho_{bl}}{\rho_{H_2O}} \right) + w_{g} x_{Na_2SO_4 fa} + x_{Na_2CO_3 fa} \right] + w_{sc} + R_{H_2S} \left( \frac{M_{CO_2}}{M_{H_2S}} - 1 \right) \]

Carbonate

\[
\frac{d}{dt} \left( \rho_{bl} V_{bl} x_{Na_2CO_3} \right) = w_{bl} \rho_{bl} x_{Na_2CO_3 fa} + w_{g} x_{Na_2CO_3 fa}
\]

\[+ R_{H_2S} \left( \frac{M_{Na_2CO_3}}{M_{H_2S}} \right) - w_{bl} x_{Na_2CO_3} \]

(157)
Substitution of (151) and (153) into (157) gives for the weight fraction of carbonate in the vat liquor

\[
\frac{d}{dt} X_{\text{Na}_2\text{CO}_3} = \frac{1}{V_{b1} \rho_{b1}} \left[ w_{b1} \left( X_{\text{Na}_2\text{CO}_3}^{(pr)} - X_{\text{Na}_2\text{CO}_3} \right) \right. \\
- \left. \left( w_{g} \left( X_{\text{Na}_2\text{S}O_4fa}^{(s)} + w_{bld} - R_{H_2O} + R_{H_2S} \frac{M_{\text{CO}_2}}{M_{H_2S}} - 1 \right) \right. \\
+ \left. w_{sc} \right) X_{\text{Na}_2\text{CO}_3} + w_{g} \left( X_{\text{Na}_2\text{CO}_3fa} \left( 1 - X_{\text{Na}_2\text{CO}_3} \right) \right) \\
+ R_{H_2S} \left( \frac{M_{\text{Na}_2\text{CO}_3}}{M_{H_2S}} \right) \right] \\
\text{(158)}
\]

Input solids

\[
\frac{d}{dt} \left( \rho_{b1} V_{b1} X_{b1s} \right) = w_{b1} X_{b1s} + w_{bld} X_{blds} \\
- R_{H_2S} \left( \frac{M_{\text{Na}_2\text{S}}}{M_{H_2S}} \right) - w_{b1} X_{b1s} \\
\text{(159)}
\]

Substitution of (151) and (153) into (159) gives for the weight fraction of input solids in the vat liquor

\[
\frac{d}{dt} X_{b1s} = \frac{1}{V_{b1} \rho_{b1}} \left[ w_{b1} \left( X_{b1s}^{(pr)} - X_{b1s} \right) \right. \\
- \left. \left( w_{g} \left( X_{\text{Na}_2\text{S}O_4fa}^{(s)} \right) \right. \\
+ \left. X_{\text{Na}_2\text{CO}_3fa} \right) - R_{H_2O} + R_{H_2S} \left( \frac{M_{\text{CO}_2}}{M_{H_2S}} - 1 \right) + w_{sc} \right) X_{b1s} \\
+ w_{bld} \left( X_{blds} - X_{b1s} \right) \right] \\
\text{(160)}
\]

Water

\[
X_{b1w} = 1 - X_{\text{Na}_2\text{S}O_4} - X_{\text{Na}_2\text{CO}_3} - X_{b1s} \\
\text{(161)}
\]
Composition of input solids

Sodium sulfide

\[
\frac{d}{dt} \left( \rho_{bl} V_{bl} X_{b|ls} X_{(bl|ce)} \right) = W_{bl} X_{b|ls} X_{Na_2S} + W_{bld} X_{b|lds} X_{Na_2S} - R_{H_2S} \left( \frac{M_{Na_2S}}{M_{H_2S}} \right) - W_{bl} X_{b|ls} X_{Na_2S} \tag{162}
\]

In the second term on the right the assumption is used that the composition of the input solids in the dilution liquor is the same as in the input solids in the strong black liquor from the precipitator.

Expansion of the left side of (162) yields

\[
\frac{d}{dt} \left( \rho_{bl} V_{bl} X_{b|ls} X_{(bl|ce)} \right) = X_{(bl|ce)} \frac{d}{dt} \left( \rho_{bl} V_{bl} X_{b|ls} \right) + (\rho_{bl} V_{bl} X_{b|ls}) \frac{d}{dt} X_{Na_2S} \tag{163}
\]

Substitution of (159) and (163) into (162) gives for the weight fraction of sodium sulfide in the vat liquor input solids

\[
\frac{d}{dt} X_{Na_2S} = \frac{1}{V_{bl} \rho_{bl} X_{b|ls}} \left[ W_{(pr)} X_{(pr)} X_{(bl|pr)} X_{Na_2S} - X_{Na_2S} \right] + W_{bld} X_{b|lds} \left[ X_{Na_2S} - X_{Na_2S} \right] - R_{H_2S} \left( \frac{M_{Na_2S}}{M_{H_2S}} \right) \left[ 1 - X_{Na_2S} \right] \tag{164}
\]
Sodium sulfide is the only component of the input solids that actually changes in the cascade evaporator. The rest of the components are present in the same ratio with respect to each other as before, but in a slightly different ratio with respect to the new total amount of input solids.

Hydrogen

\[
\frac{x_{\text{H}}^{(\text{blce})}}{1 - x_{\text{Na}_2\text{S}}^{(\text{blce})}} = \frac{x_{\text{H}}^{(\text{blpr})}}{1 - x_{\text{Na}_2\text{S}}^{(\text{blpr})}} \tag{165}
\]

\[
x_{\text{H}}^{(\text{blce})} = \frac{1 - x_{\text{Na}_2\text{S}}^{(\text{blce})}}{1 - x_{\text{Na}_2\text{S}}^{(\text{blpr})}} x_{\text{H}}^{(\text{blpr})} \tag{166}
\]

Oxygen

\[
x_{\text{O}}^{(\text{blce})} = \frac{1 - x_{\text{Na}_2\text{S}}^{(\text{blce})}}{1 - x_{\text{Na}_2\text{S}}^{(\text{blpr})}} x_{\text{O}}^{(\text{blpr})} \tag{167}
\]

Sulfur not as sodium sulfide

\[
x_{\text{S}}^{(\text{blce})} = \frac{1 - x_{\text{Na}_2\text{S}}^{(\text{blce})}}{1 - x_{\text{Na}_2\text{S}}^{(\text{blpr})}} x_{\text{S}}^{(\text{blpr})} \tag{168}
\]

Carbon

\[
x_{\text{C}}^{(\text{blce})} = \frac{1 - x_{\text{Na}_2\text{S}}^{(\text{blce})}}{1 - x_{\text{Na}_2\text{S}}^{(\text{blpr})}} x_{\text{C}}^{(\text{blpr})} \tag{169}
\]

Sodium not as sodium sulfide

\[
x_{\text{Na}}^{(\text{blce})} = 1 - x_{\text{Na}_2\text{S}}^{(\text{blce})} - x_{\text{H}}^{(\text{blce})} - x_{\text{O}}^{(\text{blce})} - x_{\text{S}}^{(\text{blce})} - x_{\text{C}}^{(\text{blce})} \tag{170}
\]
ENERGY BALANCE

Gas temperature

\[
\frac{d}{dt} \left( V_g \rho_g c_{pg} T_g \right) = w^{(s)} c_{pg} (T_g - 80) - A_{wh} U_{wh} (T_g - T_{wh}) - A_V U_V (T_g - T_{bl})
\]

\[
- w_g \left[ X(g_5) N_{Na_2SO_4}^{fa} + X(g_5) N_{Na_2CO_3}^{fa} \right] c_{pfa} (T_g - 80)
\]

\[
+ R_{H_2O} c_{pst} (T_{wh} - 80) - w_g c_{pg} (T_g - 80)
\]

On the right hand side are the heat content of the gas (and solid particles) from the economizer, the heat transferred to the cascade wheel, the heat transferred to the liquor in the vat, the heat content of the fly ash falling into the vat liquor, the heat content of the water vapor from the wheel surface, and the heat content of the gases going to the precipitator. It is assumed that the heat for evaporation is first transferred to the wheel surface, and then used for evaporation of water. When the above equation is to be made algebraic it becomes quadratic in \( T_g \), and is solved by iteration with Equation (148).

\[
T_g = \frac{1}{A_{wh} U_{wh} + A_V U_V + w_g \left[ X(g_5) N_{Na_2SO_4}^{fa} + X(g_5) N_{Na_2CO_3}^{fa} \right] c_{pfa} + w_g c_{pg}} \left[ w_g c_{pg} (T_g - 80) + A_{wh} U_{wh} (T_{wh} - 80) \right. \\
\left. + A_V U_V (T_{bl} - 80) + R_{H_2O} c_{pst} (T_{wh} - 80) \right] + 80
\]
Liquor temperature

\[
\begin{align*}
\frac{d}{dt} T_{bl} &= \frac{1}{V_{b1} \rho_{b1} c_{pb1}} \left[ w_{b1} \left( x_{blw} c_{pw} + (1 - x_{blw}) c_{pb1s} \right) T_{bl} \\
&\quad - 80 \right] + w_{bd1} \left( x_{bd1w} c_{pw} + (1 - x_{bd1w}) c_{pb1s} \right) T_{bd1} - 80 \\
&\quad + w_{sc} c_{psc} (T_{sc} - 80) + A_{wh} U_{wh} (T_{g} - T_{wh}) + A_{v} U_{v} (T_{g} - T_{bl}) \\
&\quad + w_{g} (s) \left[ x_{Na_{2}SO_{4}fa} + x_{Na_{2}CO_{3}fa} \right] c_{pf(a)} (T_{g} - 80) \\
&\quad - R_{H_{2}O} \left[ H_{H_{2}O} c_{pw} (T_{wh} - 80) \right] \\
&\quad - w_{bl} \left( x_{blw} c_{pw} + (1 - x_{blw}) c_{pb1s} \right) (T_{bl} - 80)
\end{align*}
\]

(173)

The heat content of the liquor from the precipitator, the heat content of the dilution liquor, the heat content of the makeup salt cake, the heat transferred to the wheel and the liquor in the vat respectively, the heat content of the fly ash falling into the liquor, the heat of evaporation, the heat required to raise the temperature of the evaporated water to the wheel temperature, and the heat content of the black liquor leaving the vat make up the right hand side of the equation. The energy involved in the formation of hydrogen sulfide has been neglected. \( H_{H_{2}O} \) is the heat of evaporation of water at temperature \( T_{wh} \).
The electrostatic precipitator separates most of the salt cake and carbonate particulates from the gases from the cascade evaporator. Only the wet bottom precipitator is considered here. In the wet bottom precipitator the black liquor from the multiple effect evaporators is circulated so that it can pick up the particulates that have been separated from the gases. The particulates are then brought back to the furnace with the liquor. Very little exchange of heat takes place between the liquor and the gases. Normally the temperature of the gases are above the dew point. If condensation should occur, then the rate of corrosion of the precipitator will increase due to the presence of sulfurous compounds.

The operating parameters of the precipitator are usually fixed. The efficiency will vary with the gas flow, decreasing with increasing flow, [22, pp. 168]. The power requirements for precipitation are negligible [22, pp. 196].

The main assumptions are:
1. The liquor in the precipitator bottom is perfectly mixed.
2. No evaporation, chemical reaction or heat exchange takes place. The temperatures of the gas and the liquor entering the precipitator are the same as the temperatures of the gas and the liquor leaving the precipitator.
Equations for the energy and material balance are:

(The superscript (pr) on \( w_g, \rho_{bl}, V_{bl}, w_{bl} \), and the \( X_i \), and
the superscript (gpr) on the \( X_i \) have been omitted.)

**MATERIAL BALANCE FOR GAS**

Salt cake particulates

\[
\begin{align*}
\rho_{g} X_{\text{Na}_2\text{SO}_4} &= (1 - K_p (e)) \rho_{g} X_{\text{Na}_2\text{SO}_4}(c) \\
K_p &= \text{the precipitator efficiency coefficient defined as the ratio between the precipitated particulates and the incoming particulates in the gas. It is usually between 0.9 and 1.0.}
\end{align*}
\]

Precipitator efficiency

\[
K_p = 1 - \exp\left(-\frac{1}{w_{g}(e)(1 - X_{\text{Na}_2\text{SO}_4}(c) - X_{\text{Na}_2\text{CO}_3}(c))}\right)
\]

\(K_{pe}\) is determined by the fixed operating parameters of the precipitator as electrode voltage, baffle arrangement, precipitator volume, and rapping frequency. The dependence of \(K_{pe}\) on gas flow is taken from [22, pp. 168].

Carbonate particulates

\[
\begin{align*}
\rho_{g} X_{\text{Na}_2\text{CO}_3} &= (1 - K_p) \rho_{g} X_{\text{Na}_2\text{CO}_3}(c) \\
\end{align*}
\]

Sulfur dioxide

\[
\begin{align*}
\rho_{g} X_{\text{SO}_2} &= \rho_{g} X_{\text{SO}_2}(c) \\
\end{align*}
\]
Hydrogen sulfide
\[ w_g X_{H_2S} = w_{(ce)} X_{(gce)}^{(H_2S)} \quad (178) \]

Carbon monoxide
\[ w_g X_{CO} = w_{(ce)} X_{(gce)}^{(CO)} \quad (179) \]

Carbon dioxide
\[ w_g X_{CO_2} = w_{(ce)} X_{(gce)}^{(CO_2)} \quad (180) \]

Water
\[ w_g X_{H_2O} = w_{(ce)} X_{(gce)}^{(H_2O)} \quad (181) \]

Nitrogen
\[ w_g X_{N_2} = w_{(ce)} X_{(gce)}^{(N_2)} \quad (182) \]

Oxygen
\[ w_g X_{O_2} = w_{(ce)} X_{(gce)}^{(O_2)} \quad (183) \]

Total flow of gas and particulates from the precipitator
\[ w_g = w_{(ce)} \left[ 1 - K_{pe} \left( X_{(gce)}^{(Na_2SO_4p)} + X_{(gce)}^{(Na_2CO_3p)} \right) \right] \quad (184) \]
MATERIAL BALANCE FOR THE BLACK LIQUOR IN THE PRECIPITATOR BOTTOM

Salt cake

\[ \frac{d}{dt} (\rho_{bl} V_{bl} X_{Na_2SO_4}) = w_{bl} X_{(pi)} + K_{pe} \omega_g X_{Na_2SO_4 p} - w_{bl} X_{Na_2SO_4} \]  \hspace{1cm} (185)

The flow of salt cake in the liquor entering the precipitator (this is usually zero), the salt cake flow due to precipitation, and the salt cake in the liquor leaving the precipitator bottom for the cascade evaporator represent the total number of contributions to the salt cake material balance.

Liquor total mass

\[ \frac{d}{dt} (\rho_{bl} V_{bl}) = w_{bl} + K_{pe} \omega_g \left( X_{Na_2SO_4 p} + X_{Na_2CO_3 p} \right) - w_{bl} \]  \hspace{1cm} (186)

The three entries are the flow of liquor into the precipitator, the flow of precipitate, and the flow of liquor leaving the precipitator.

Total liquor flow from the precipitator.

As the volume of the liquor bottom \( V_{bl} \) is constant, the volumetric flow of liquor flow out must equal the volumetric flow in, - if shrinkage due to mixing is neglected.
The volume flow of the precipitate is neglected and it is assumed that it dissolves in the liquor without changing the liquor volume. The equation for the liquor volume flow rate from the precipitator bottom

\[
\frac{w_{bl}}{\rho_{bl}} = \frac{w_{(pi)}}{\rho_{(pi)}} \quad (187)
\]

The mass flow of liquor from the precipitator bottom is then

\[
w_{bl} = \frac{\rho_{bl}}{\rho_{(pi)}} \cdot w_{(pi)} \quad (188)
\]

Expansion of the left side of (2.185) yields

\[
\frac{d}{dt} (\rho_{bl} V_{bl} x_{Na_2SO_4}) = V_{bl} \left[ \rho_{bl} \frac{d}{dt} x_{Na_2SO_4} + x_{Na_2SO_4} \frac{d}{dt} \rho_{bl} \right] \quad (189)
\]

By substituting (189) and (186) into (185) the equation becomes for the weight fraction of salt cake in the bottom liquor

\[
\frac{d}{dt} x_{Na_2SO_4} = \frac{1}{V_{bl} \rho_{bl}} \left[ w_{(pi)} x_{(pi)} \left( x_{Na_2SO_4} - x_{Na_2SO_4} \right) 
+ K_{pe} w_{(ce)} x_{(gce)} p_{Na_2SO_4}
- K_{pe} w_{(ce)} \left( x_{(gce)} + x_{(gce)} p_{Na_2CO_3} \right) x_{Na_2SO_4} \right] \quad (190)
\]
Equation (188) into (186) gives for the liquor density
\[
\frac{d}{dt} \rho_{bl} = \frac{1}{V_{bl}} \left[ w_{bl}(pi) \left( 1 - \frac{\rho_{bl}}{\rho_{pi}} \right) \right]
\]
\[+ K_{pe} w_g(ce) \left( x_{(gce)} + x_{(gce)}^{Na_2CO_3} \right) \]

(191)

Carbonate
\[
\frac{d}{dt} \left( \rho_{bl} \ V_{bl} \ x_{Na_2CO_3} \right) = w_{bl}(pi) \ x_{Na_2CO_3}^{pi}
\]
\[+ K_{pe} w_g(ce) \ x_{Na_2CO_3}^{gce} - w_{bl} \ x_{Na_2CO_3} \]

(192)

Substitution of (186) into (192) gives for the weight fraction of carbonate in the liquor
\[
\frac{d}{dt} x_{Na_2CO_3} = \frac{1}{V_{bl} \ \rho_{bl}} \left[ w_{bl}(pi) \ x_{Na_2CO_3}^{pi} - x_{Na_2CO_3} \right]
\]
\[+ K_{pe} w_g(ce) \ x_{Na_2CO_3}^{gce} \]
\[+ x_{Na_2CO_3} \left( x_{Na_2SO_4}^{(gce)} + x_{Na_2CO_3}^{(gce)} \right) \]

(193)

Input solids
\[
\frac{d}{dt} \left( \rho_{bl} \ V_{bl} \ x_{bls} \right) = w_{bl}(pi) \ x_{bls}^{pi} - w_{bl} \ x_{bls} \]

(194)

Substitution of (186) into (194) gives for the weight fraction of input solids in the liquor
\[
\frac{d}{dt} x_{b\text{ls}} = \frac{1}{V_{b\text{l}} \rho_{b\text{l}}} \left[ w_{b\text{l}} (p_{\text{i}}) (x_{\text{b\text{l}s}} - x_{b\text{ls}}) \right] \\
- K_{pe} w_{g}^{(ce)} \left[ x_{(\text{gce})} \left( X_{Na_{2}SO_{4}P} + X_{Na_{2}CO_{3}P} \right) x_{b\text{l}s} \right]
\] (195)

Water

\[
x_{b\text{l}w} = 1 - X_{Na_{2}SO_{4}} - X_{Na_{2}CO_{3}} - x_{b\text{l}s}
\] (196)
GENERAL

A detailed description of the use of this model to develop the parameters for a particular furnace is given in the separate Report on this portion of the Chemical and Energy Recovery Unit [32] which has been transmitted separately to the supporting companies.
LIST OF SYMBOLS USED

Superscripts are used to indicate to which subsection of the furnace the variables belong.

Special subscripts are used to indicate the physical component to which the variable refers.

As an example, $w_{bl}^{(sp)}$ is the flow (w) of black liquor (bl) through a spray nozzle (sp).

In the following the main symbols are listed first, then the superscripts, and finally the special subscripts.

MAIN SYMBOLS

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>Area (ft$^2$)</td>
</tr>
<tr>
<td>$A_{ecmx}$</td>
<td>Maximum area of economizer (ft$^2$)</td>
</tr>
<tr>
<td>$A_f$</td>
<td>Furnace crosssectional area (ft$^2$)</td>
</tr>
<tr>
<td>c</td>
<td>Concentration (%)</td>
</tr>
<tr>
<td>$c_p$</td>
<td>Specific heat (Btu/(lb)(°F))</td>
</tr>
<tr>
<td>C</td>
<td>Cost ($/lb)</td>
</tr>
<tr>
<td>F</td>
<td>Combustion air availability</td>
</tr>
<tr>
<td>h</td>
<td>Char bed height (ft)</td>
</tr>
<tr>
<td>H</td>
<td>Enthalpy, Heat of reaction (Btu/lb)</td>
</tr>
<tr>
<td>J</td>
<td>Performance measure ($/Btu)</td>
</tr>
<tr>
<td>$K_{at}$</td>
<td>Total combustion air gain (lb/Btu)</td>
</tr>
<tr>
<td>$K_{a1}$</td>
<td>Primary combustion air gain (lb/Btu)</td>
</tr>
</tbody>
</table>
\[ \Delta K_{\text{a1}} \] Primary combustion air gain increment (lb/Btu)

\[ K_{\text{cl}} \] Liquor temperature controller gain (°F/hr)

\[ K_{\text{cm}} \] Char bed reaction rate coefficient (lb/hr)

\[ K_{\text{CO}} \] CO formation rate coefficient

\[ K^{(1)}_{\text{g}} \] Oxygen deficiency parameter

\[ K_{\text{H2O}} \] Mass transfer coefficient (lb/(ft²)(°F)(hr))

\[ K^{(\text{ce})}_{\text{H2S}} \] H₂S formation rate coefficient (lb/(ft²)(hr))

\[ K^{(\text{g2})}_{\text{H2S}} \] H₂S formation rate coefficient

\[ K_{\text{I}} \] Digital control algorithm integration gain

\[ K_{\text{p}} \] Digital control algorithm proportional gain

\[ K_{\text{pa}} \] Primary combustion air gain

\[ K_{\text{pe}} \] Precipitator efficiency

\[ K_{\text{po}} \] Secondary air port coefficient ((ft²)(hr)/lb)

\[ K_{\text{SO2}} \] SO₂ formation rate coefficient

\[ K_{\text{ta}} \] Total combustion air gain

\[ K_{\text{1pe}} \] Precipitator parameter (lb/hr)

\[ m \] Mass (lb)

\[ M \] Atomic or molecular weight

\[ n \] Index

\[ N \] Number of spray nozzles

\[ \dot{Q} \] Heat flow (Btu/hr)

\[ \dot{Q}_{\text{L}} \] Heat loss (Btu/hr)

\[ \dot{Q}^{(c)}_{\text{t}} \] Total available combustion energy of reacting char (Btu/hr)

\[ \dot{Q}^{(\text{cb})} \] Combustion energy released in the char bed (Btu/hr)
\[ \dot{Q}(c_1) \] Combustion energy released in primary zone and char bed (Btu/hr)

\[ \dot{Q}(c) \] Combustion energy released in primary zone above the char bed (Btu/hr)

\[ R \] Reaction rate (lb/hr)

\[ t \] time (hr)

\[ t_{\text{delay}} \] Time delay in CHRCNT (char bed control program) (hr)

\[ t_{\text{per}} \] Time delay in CHRCNT (hr)

\[ t_1 \] Time delay in PRIGN (primary air gain program) (hr)

\[ t_2 \] Time delay in PRIGN (hr)

\[ T \] Temperature (°F)

\[ \Delta T_{\text{bl1}} \] Parameter in CHRCNT (°F)

\[ T_{\text{bl1}} \] Spray droplet distribution parameter (°F)

\[ T_{\text{bl2}} \] Spray droplet distribution parameter (°F)

\[ T_{\text{bl3}} \] Spray droplet distribution parameter (°F)

\[ T_{\text{blmix}} \] Parameter in CHRCNT (°F)

\[ T_{\text{cmin}} \] Char bed temperature limit (°F)

\[ T_{\text{hi}} \] Higher band temperature in CHRCNT (°F)

\[ \Delta T_{\text{li}} \] Temperature band width in CHRCNT (°F)

\[ T_{\text{lo}} \] Lower band temperature in CHRCNT (°F)

\[ T_{\text{imin}} \] Parameter in PRIGN (°F)

\[ T_{\text{lr}} \] Black liquor "roping" temperature (°F)

\[ \Delta T_{\text{lst}} \] Parameter in CHRCNT (°F)

\[ T_1 \] Parameter in PRIGN (°F)

\[ u \] Velocity (ft/hr)

\[ u_{g_1} \] Maximum primary combustion gas velocity (ft/hr)
$U_r$ Radiation heat transfer coefficient
\[(\text{Btu}/(\text{ft}^2)(\text{o}R^4)(\text{hr}))\]

$U_{rl}$ Linearized radiation heat transfer coefficient
\[(\text{Btu}/(\text{ft}^2)(\text{o}F)(\text{hr}))\]

$v$ Velocity (ft/sec)

$V$ Volume (ft$^3$)

$V_p$ Pseudo volume (ft$^3$)

$w$ Mass flow (lb/hr)

$w_{as}$ Primary air flow set point (lb/hr)

$w_{atff}$ Feedforward computed total air flow (lb/hr)

$w_{ats}$ Total air flow set point (lb/hr)

$w_h$ "Higher heat value" flow (lb/hr)

$\Delta w_{O_2}a$ Feedback correction to total air flow (lb/hr)

$w^{(t)}_o$ Required oxygen flow for complete combustion in primary zone (lb/hr)

$X$ Mass fraction (lb/lb)

$Y_1$ Fraction of liquor spray equal to or larger than 500 μm

$Y_2$ Fraction of liquor spray equal to or smaller than 10 μm

$\alpha$ Filter coefficient for air control system

$\alpha_c$ Reaction rate coefficient for the char bed (°R)

$\alpha_{CO}$ Turbulence CO generation rate coefficient for ZONE2 (secondary zone program) \((\text{ft})(\text{sec})^2/\text{lb}\)

$\alpha_{H_2S}$ Turbulence $H_2S$ generation rate coefficient for ZONE2 \((\text{ft})(\text{sec})^2/\text{lb}\)
\( \alpha_{SO_2} \) Turbulence \( SO_2 \) generation rate coefficient for ZONE2 \((\text{ft})(\text{sec})^2/\text{lb})

\( \beta_{CO} \) Oxygen concentration \( CO \) generation rate coefficient for ZONE2

\( \beta_{H_2S} \) Oxygen concentration \( H_2S \) generation rate coefficient for ZONE2

\( \beta_{SO_2} \) Oxygen concentration \( SO_2 \) generation rate coefficient for ZONE2

\( \delta \) Turbulence function in ZONE2 \((\text{lb}/(\text{ft})(\text{sec})^2))

\( \Delta \) Oxygen excess/deficiency function in CHRBED (%)

\( \eta_{ecmn} \) Economizer damping ratio lower limit

\( \eta_r \) Smelt reduction ratio

\( \eta_1 \) Primary zone entrainment ratio

\( \eta(c) \) Char bed combustion energy ratio

\( \rho \) Density \((\text{lb}/\text{ft}^3))

**SUPERSCRIPrTS**

\( a_1 \) Primary combustion air

\( a_2 \) Secondary combustion air

\( b_1 \) Black liquor input solids

\( b_{1ce} \) Black liquor input solids from the cascade evaporator

\( b_{1pr} \) Black liquor input solids from the precipitator

\( c_b \) Char bed

\( c_e \) Cascade evaporator

\( c_m \) Reacting char

\( c_s \) Char bed surface
-305-

dg₂  Dry gas in secondary zone

gce  Gas from the cascade evaporator

gpr  Gas from the precipitator

g₁   Gas from the primary zone

g₂   Gas from the secondary zone

g₃   Gas from the superheater zone

g₄   Gas from the boiler zone

gₛ   Gas from the economizer zone

h    Black liquor heater

pe   Primary zone entrainment

pi   Precipitator input from multiple-effect evaporators

pr   Precipitator

sm   Smelt

sp   Spray nozzles

spc  Fraction of spray not entrained in the primary zone

₁   Primary zone

₂   Secondary zone

₃   Superheater zone

₄   Boiler zone

₅   Economizer zone

SUBSCRIPTS

a   Combustion air

b   Boiler, boiler water

bd  Blow down
<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>bl</td>
<td>Black liquor</td>
</tr>
<tr>
<td>bld</td>
<td>Weak black liquor for dilution</td>
</tr>
<tr>
<td>blds</td>
<td>Input solids in &quot;dilution&quot; black liquor</td>
</tr>
<tr>
<td>bldw</td>
<td>Water in &quot;dilution&quot; black liquor</td>
</tr>
<tr>
<td>bls</td>
<td>Black liquor input solids</td>
</tr>
<tr>
<td>blts</td>
<td>Black liquor total solids</td>
</tr>
<tr>
<td>blw</td>
<td>Water in black liquor</td>
</tr>
<tr>
<td>c</td>
<td>Char bed, convective heat transfer</td>
</tr>
<tr>
<td>C</td>
<td>Carbon, carbon not as Na$_2$CO$_3$</td>
</tr>
<tr>
<td>C(Na$_2$CO$_3$)</td>
<td>Carbon as Na$_2$CO$_3$</td>
</tr>
<tr>
<td>CO</td>
<td>Carbon monoxide</td>
</tr>
<tr>
<td>CO$_2$</td>
<td>Carbon dioxide</td>
</tr>
<tr>
<td>dw</td>
<td>Desuperheater water</td>
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<tr>
<td>ec</td>
<td>Economizer tube bank</td>
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<td>Gas</td>
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<td>Hydrogen</td>
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<td>Water</td>
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<td>Hydrogen sulfide</td>
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<td>i</td>
<td>Index, input</td>
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<td>ia</td>
<td>Infiltration air</td>
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<td>Index</td>
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<td>N</td>
<td>Nitrogen</td>
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<td>N$_2$</td>
<td>Nitrogen gas</td>
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<td>Sodium</td>
</tr>
<tr>
<td>Nap</td>
<td>Sodium in particulates</td>
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<tr>
<td>Na$_2$CO$_3$</td>
<td>Sodium carbonate</td>
</tr>
<tr>
<td>Symbol</td>
<td>Description</td>
</tr>
<tr>
<td>----------</td>
<td>-----------------------------------</td>
</tr>
<tr>
<td>Na\textsubscript{2}CO\textsubscript{3}fa</td>
<td>Sodium carbonate fly ash</td>
</tr>
<tr>
<td>Na\textsubscript{2}CO\textsubscript{3}p</td>
<td>Sodium carbonate particulates</td>
</tr>
<tr>
<td>Na\textsubscript{2}S</td>
<td>Sodium sulfide</td>
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<tr>
<td>Na\textsubscript{2}SO\textsubscript{4}</td>
<td>Sodium sulfate (salt cake)</td>
</tr>
<tr>
<td>Na\textsubscript{2}SO\textsubscript{4}fa</td>
<td>Sodium sulfate fly ash</td>
</tr>
<tr>
<td>Na\textsubscript{2}SO\textsubscript{4}p</td>
<td>Sodium sulfate particulates</td>
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<tr>
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<td>Oxygen</td>
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<td>O\textsubscript{2}</td>
<td>Oxygen gas</td>
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<td>r</td>
<td>Reduction, radiation</td>
</tr>
<tr>
<td>sb</td>
<td>Soot blowing steam</td>
</tr>
<tr>
<td>sc</td>
<td>Salt cake (Na\textsubscript{2}SO\textsubscript{4})</td>
</tr>
<tr>
<td>sh</td>
<td>Superheater</td>
</tr>
<tr>
<td>sm</td>
<td>Smelt</td>
</tr>
<tr>
<td>st</td>
<td>Steam</td>
</tr>
<tr>
<td>S</td>
<td>Sulfur, sulfur not as Na\textsubscript{2}SO\textsubscript{4}</td>
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<td>S(Na\textsubscript{2}SO\textsubscript{4})</td>
<td>Sulfur as Na\textsubscript{2}SO\textsubscript{4}</td>
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<tr>
<td>SO\textsubscript{2}</td>
<td>Sulfur dioxide</td>
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<td>t</td>
<td>Total</td>
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<tr>
<td>v</td>
<td>Cascade evaporator vat</td>
</tr>
<tr>
<td>w</td>
<td>Water</td>
</tr>
<tr>
<td>wh</td>
<td>Cascade evaporator wheel</td>
</tr>
<tr>
<td>wv</td>
<td>Water vapor</td>
</tr>
</tbody>
</table>
REFERENCES CITED


31. Aiken, P. M. and Smith, C. C., Operating Manual for the Purdue Hybrid Computer Facility, Purdue Laboratory for Applied Industrial Control, Purdue University, Lafayette, Indiana 47907, October 1969.

SECTION VII

MATHEMATICAL MODEL OF SLAKING/CAUSTICIZING
AND SOLIDS SETTLING

INTRODUCTION

The primary functions of the recausticizing process within the kraft pulping chemical recovery process may be summarized as follows (2):

1. To convert as much of the recovered sodium carbonate to sodium hydroxide as possible.
2. To produce a suitably clarified white liquor of the required concentration.
3. To separate, wash, and dewater the calcium carbonate (CaCO₃) mud suitably to prepare it for calcination.
4. To clarify the green liquor prior to recausticizing and to wash the resulting dregs.

Item 1 above is performed by a slaking/causticizing reaction. Items 2, 3, and 4 are performed primarily by the settling of suspended solid particles in a liquid medium. It is the purpose of this Section to mathematically describe the basic dynamic behavior of the slaking/causticizing and solids settling processes. This model can be used to establish what the most critical process input and output variables are, and how they can be used in a dynamic control scheme for improving the overall performance of the recovery system.
A flow diagram for a typical kraft pulp mill liquor preparation system is shown in Figure 1. The smelt production of the recovery furnace is the primary forcing variable for this system. The smelt is dissolved and is transferred via density control to a clarifier. The solution containing the dissolved smelt is referred to as green liquor. It is made up primarily of sodium carbonate (Na₂CO₃) and sodium sulfide (Na₂S) and some suspended solids such as carbon particles, iron compounds, and pieces of refractory lining, which are all picked up by the smelt in the recovery furnace. These suspended solids, which are called dregs, must be removed, or they will mechanically and/or chemically mix and react with CaCO₃ mud (formed subsequently in the causticizing reaction), resulting in a steadily increasing accumulation of inert material which decreases the availability of the recalcined lime. Thus, a green liquor clarifier is needed. The green liquor clarification process is similar to that of white liquor, so a detailed discussion and derivation of the process dynamics will be deferred until the discussion of white liquor clarification and solids settling.

From the clarifier the green liquor is pumped to a storage tank. From the storage tank it is transferred via flow and temperature control to the slaking/causticizing tanks.
FIGURE 1

UNIT OPERATION FLOWSHEET FOR A

CONVENTIONAL LIQUOR PREPARATION SYSTEM
SI ALKING/CAUSTICIZING

The purpose of the slaking/causticizing process is to convert the Na$_2$CO$_3$ in the green liquor to sodium hydroxide (NaOH) to produce white liquor. (The Na$_2$S content remains essentially unchanged.) The reaction proceeds in two stages. The first stage reaction, known as slaking, involves the addition of quick-lime (CaO) to green liquor where it reacts with the water to form calcium hydroxide, Ca(OH)$_2$, and heat. The reaction may be written as follows:

$$\text{CaO} + \text{H}_2\text{O} \longrightarrow \text{Ca(OH)}_2 + 486 \text{ B.t.u. per lb. CaO}$$

In the second stage, the Ca(OH)$_2$ which was formed in slaking reacts with Na$_2$CO$_3$ as written in the following chemical equation:

$$\text{Ca(OH)}_2 + \text{Na}_2\text{CO}_3 \xrightarrow{K} 2 \text{NaOH} + \text{CaCO}_3$$

Although the reactions are written in two stages, they actually overlap because part of the causticizing occurs almost coincidentally with the slaking. The causticizing reaction is reversible and thus proceeds in either direction depending on the relative concentrations of the reactants and products. Because the CaCO$_3$ is less soluble than the Ca(OH)$_2$, the causticizing reaction proceeds to the right. However, because of the reversibility, all of the Na$_2$CO$_3$ cannot be converted to NaOH regardless of the amount of lime used. The extent of conversion is called causticizing efficiency (C.E.) and is defined as

$$\text{C.E.} = \frac{\text{NaOH}}{\text{NaOH} + \text{Na}_2\text{CO}_3} \times 100 \% \ (\text{expressed as Na}_2\text{O})$$
The causticizing efficiency depends on the concentration of sodium compounds in the green liquor entering the slaker. Lower concentrations produce higher conversion, because in stronger solutions the NaOH progressively reduces the solubility of Ca(OH)$_2$. This continues until there are not enough calcium ions present to exceed the solubility limit of CaCO$_3$.

Another factor which lowers the causticizing efficiency in practice is the presence of Na$_2$S in the green liquor. The mechanism causing this phenomenon is not completely understood. A probable explanation is that Na$_2$S, because it is more basic than Na$_2$CO$_3$, hydrolyzes to a considerable degree according to the following:

\[
\text{Na}_2\text{S} + \text{H}_2\text{O} = \text{NaOH} + \text{NaHS}
\]

The hydroxyl ions produced tend to suppress the causticization of Na$_2$CO$_3$. A typical curve obtained using experimental data which shows the effects of green liquor concentration and of green liquor sulfidity* on causticizing efficiency is shown in Figure 2. Because the mechanism of the effect of Na$_2$S on causticization has not been established, it will be taken into account in the model by the relationship shown in the graph of Figure 2 and other sources of empirical data.

The equipment involved in the slaking/causticizing process is shown diagrammatically in Figures 1 and 3. The slaker is

---

*Percent sulfidity is defined as $\frac{\text{Na}_2\text{S}}{\text{NaOH} + \text{Na}_2\text{S}} \times 100\%$ (expressed as Na$_2$O).
FIGURE 2

EFFECT OF SULFIDITY ON CAUSTICIZING EFFICIENCY
FIGURE 3

HARDWARE CONFIGURATION OF A TYPICAL
SLAKER USED IN THE KRAFT RECOVERY SYSTEM
essentially an agitated reaction vessel of the continuous type. The reacting slurry flows to a non-agitated classifying zone from the slaking compartment where coarse solids (grits) settle out and are slowly conveyed up the incline by rakes. The grits are washed once they are out of the slurry pool, and are discharged to waste. The reacting slurry overflows a weir in the classifier and is transferred to the causticizing tanks. There are usually three of these tanks in series. They are identical in design. They are simple, stirred tank continuous reactors. Because the slaking and causticizing reactions occur simultaneously, the chemical kinetic equations for the slaker and the subsequent causticizers will be almost identical. The following assumptions and stipulations are made for the approximate model:

1. Perfect mixing
2. Energy input due to agitation is negligible.
3. Water evaporation is constant.
4. Material concentrations will be expressed as fractions of total sodium present because the total amount of sodium remains unchanged.
5. Only the slaking and causticizing reactions will be considered.
6. Heat loss due to radiation and convection is constant.

Let the mass fractions of \( \text{CaO}, \text{Ca(OH)}_2, \text{Na}_2\text{CO}_3, \text{NaOH}, \) and \( \text{CaCO}_3 \) be denoted by \( x_{\text{CaO}}^{(c)}, x_{\text{Ca(OH)}_2}^{(c)}, x_{\text{Na}_2\text{CO}_3}^{(c)}, x_{\text{NaOH}}^{(c)}, \) and \( x_{\text{CaCO}_3}^{(c)} \), respectively.
Applying Arrhenius' law and the mass conservation law we have for a given reactant, X, in a stirred tank reactor:

Rate of accumulation of X in reactor = (Amount of X in feed - Amount of X in the product - Amount of X used up in the reaction)

Thus for CaO from slaking:

\[
V \frac{d}{dt} \left[ \rho w_1 X_{CaO} \right] = W_{CaO} \cdot ADTP - W_{w_1} \cdot x_{CaO} \cdot ADTP - K_i \rho w_1 x_{CaO}
\]

(1)

For Ca(OH)\textsubscript{2} from slaking and causticizing:

\[
V \frac{d}{dt} \left[ \rho w_1 X_{Ca(OH)\textsubscript{2}} \right] = -W_{w_1} \cdot x_{Ca(OH)\textsubscript{2}} \cdot ADTP + K_i \rho w_1 x_{CaO} - K_{2r} \rho w_1 x_{Ca(OH)\textsubscript{2}} x_{Na_2CO_3} + K_{2r} \rho w_1 \cdot x_{NaOH} x_{CaCO_3}
\]

(2)

For Na\textsubscript{2}CO\textsubscript{3} from causticizing:

\[
V \frac{d}{dt} \left[ \rho w_1 X_{Na_2CO_3} \right] = W_{gl_1} \cdot x_{Na_2CO_3} \cdot ADTP - W_{w_1} \cdot x_{Na_2CO_3} \cdot ADTP - K_{2r} \rho w_1 x_{Ca(OH)\textsubscript{2}} x_{Na_2CO_3} + K_{2r} \rho w_1 \cdot x_{NaOH} x_{CaCO_3}
\]

(3)
For NaOH from causticizing:

\[
\frac{d}{dt} \left[ \rho_{wl} x_{\text{NaOH}}(c) \right] = -w_{wl_0}(c) \cdot x_{\text{NaOH}}(c) \cdot \text{ADTP} \\
+ K_{2r} V_p(c) x_{\text{Ca(OH)}_2}(c) x_{\text{Na}_2\text{CO}_3}(c) \\
- 2K_{2r} V_p(c) x(c)^2 x(c) \\
(4)
\]

For CaCO\textsubscript{3} from causticizing:

\[
\frac{d}{dt} \left[ \rho_{wl} x_{\text{CaCO}_3}(c) \right] = -w_{wl_0}(c) \cdot x_{\text{CaCO}_3}(c) \cdot \text{ADTP} \\
+ K_{2r} V_p(c) x_{\text{Ca(OH)}_2}(c) x_{\text{Na}_2\text{CO}_3}(c) \\
- K_{2r} V_p(c) x(c)^2 x(c) \\
(5)
\]

For total white liquor:

\[
\frac{d}{dt} \left[ \rho_{wl} \right] = \left( w_{gl_1}(c) - w_{wl_0}(c) \right) \cdot \text{ADTP} \\
(6)
\]

For water:

\[
\frac{d}{dt} \left[ \rho_{wl} x_{\text{H}_2\text{O}}(c) \right] = \left( g_{gl_1} - w_{wl_0} \right) \cdot \text{ADTP} \\
- w_{wl_0}(c) \cdot x_{\text{H}_2\text{O}}(c) \cdot \text{ADTP} - E_{\text{H}_2\text{O}} \\
(7)
\]

Therefore the total flow will be

\[
w_T(c) = w_{wl}(c) \left( x_{\text{H}_2\text{O}}(c) + x_{\text{CaO}}(c) + x_{\text{Ca(OH)}_2}(c) + x_{\text{Na}_2\text{CO}_3}(c) \\
+ x_{\text{NaOH}}(c) + x_{\text{CaCO}_3}(c) + x_{\text{Na}_2\text{S}}(c) \right) \\
(8)
\]
where

- \( \text{ADTP} \) = Pulp production (tadp/hr)
- \( \text{EH}_{2}O \) = Rate of water evaporation (lb/hr)
- \( V \) = Volume of mixture in tank (ft\(^3\))
- \( W_{\text{CaO}} \) = Input CaO Flow (lb/tadp)
- \( W_{\text{gl}} \) = Input green liquor flow (lb/tadp)
- \( W_{\text{w}} \) = Flow of white liquor (lb/tadp)
- \( W_{\text{wot}} \) = Output white liquor flow (lb/tadp)
- \( W_{\text{T}} \) = Total flow (lb/tadp)
- \( X_{\text{CaO}} \) = Mass fraction of CaO to white liquor (lb/lb), etc.
- \( \rho_{\text{w}} \) = Density of white liquor in mixture (lb/ft\(^3\))

The rate constants are defined as:

\[
K_1 = A_1 \exp \left( \frac{\Delta E_1}{RT} \right)
\]

\[
K_2 = A_2 \exp \left( \frac{\Delta E_2}{RT} \right) = \frac{K_2r}{K_2l}
\]

where

- \( A_1, A_2 \) = Arrhenius rate constant coefficients (ft\(^3\)/lb-hr)
- \( K_2r \) = Rate constant for the right directed causticizing reaction
- \( K_2l \) = Rate constant for the left directed causticizing reaction
- \( R \) = Universal gas constant (B.t.u./mole-°R)
- \( T \) = Temperature in the reactor (°R)
- \( \Delta E_1, \Delta E_2 \) = Activation energy (B.t.u./mole)
The law of the conservation of energy around the reactor is stated as:

Rate of energy accumulation in reactor =
(energy in - energy out + net energy generated by the reaction)

Thus the energy balance equation for the slaker can be written as:

\[ m c_p \frac{dT}{dt} = W(T) \cdot c_p \cdot T \cdot ADTP + W_{CaO} \cdot c_{CaO} \cdot T_{CaO} \cdot ADTP - W_{T_0} \cdot c_p \cdot T \cdot ADTP - E_{H_2O} + Q_L + K_1 H_1 V_p^{(c)} x^{(c)}_{CaO}
- K_2 H_2 V_p^{(c)} x^{(c)}_{Ca(OH)_2 x^{(c)}}_{Na_2CO_3} \]

(9)

where

- \( c_p \) = Specific heat of mixture (lb)
- \( c_{CaO} \) = Specific heat of input CaO (B.t.u./lb-°R)
- \( c_p \) = Specific heat of input liquor (B.t.u./lb-°R)
- \( H_1 \) = Heat of slaking reaction (B.t.u./lb)
- \( H_2 \) = Heat of causticizing reaction (B.t.u./lb)
- \( H_{H_2O} \) = Heat of vaporization of water (B.t.u./lb)
- \( m \) = Total mass of mixture (lb)
- \( Q_L \) = Heat loss (B.t.u./hr)
- \( T \) = Temperature of mixture (°R)
\[ T_{\text{CaO}} = \text{Temperature of input CaO (°R)} \]
\[ T_I = \text{Temperature of input liquor (°R)} \]
\[ W_{I(c)}^{(c)} = \text{Input total flow of liquor (lb/hr)} \]
\[ W_{T_o}^{(c)} = \text{Output total flow (lb/hr)} \]

Another aspect of the slaking/causticizing process which is just as important as the causticizing conversion, from a practical point of view, is the settleability of the CaCO\(_3\) precipitate (lime mud) produced (References 4,5,6,7). To begin with, the settling rate of the lime mud has a direct effect on the white liquor clarity. Secondly, because lime recovery (calcining) is an integral part of the liquor preparation system, particularly the slaking/causticizing process, the degree of preparation of lime mud for calcining is ultimately reflected back to the slaking/causticizing process. The degree of preparation is mainly dependent upon the lime mud particle size, as will be shown later.

The following discussion concerns conventional gravity sedimentation for separation of white liquor and carbonate mud. It is possible to substitute a continuous belt filter for this clarifier. Such a belt filter, as described in the overall steady-state model for the Consolidated Mill as discussed in Section III, is a much simpler simulation and control problem than the gravity clarifier described in this Section.

Poor-settling lime is difficult to wash and dewater. Already in the white liquor clarification, poorly-settled mud will naturally result in more caustic liquor being withdrawn with the mud
in the underflow of the clarifier. The caustic soda content of the mud must be reduced to a low level (usually less than 1%), or severe ring and ball formation will occur in the mud reburning process. Typically, the lime mud is washed in a sedimentation unit similar to the white liquor clarifier. Here again, a poorly-settled mud will result in a higher water content and a higher soda content underflow mud. Finally, the poor-settling mud is transferred to a vacuum filter. This filter does the final washing and dewatering of the lime mud. As mentioned previously, there is a strong relationship between settleability and lime mud particle size, the smaller particles being harder to settle. These small particles also cause "blinding" of the filter passages. Thus the shower water applied to the filter drum cannot penetrate the mud filter properly, and, in addition, the vacuum dewatering process is retarded. Hence the kiln receives a mud that has a higher moisture content and a higher soda content. The result is inefficient kiln operation on both counts.

The lime mud settling rate can be approximated by using Stoke's law. It assumes slow settling speeds, viscous friction between the mud particles and the liquid, and independent settling of spherical particles of up to 0.1 mm. in diameter. These stipulations generally agree with the conditions occurring in lime mud settlers. Stoke's law is stated as

\[ u = \frac{D^2(\rho_s - \rho_l)}{\mu} \]  

(10)
As is obvious from Equation (10), the particle size has a strong influence on the settling rate. Furthermore, the settling rate is increased by reducing the viscosity of the liquid. One can surmise that viscosity reduction is attained by raising the temperature and by lowering the concentration of the liquid. In addition, Equation (10) shows that by decreasing the density of the liquid relative to that of the mud, an increase in settling rate will result. Therefore, some degree of control of the mud settling rate can be exercised by liquor temperature control and by liquor concentration control.

With regard to dynamic modeling of the settler process, one can see that it would be desirable to have some way of quantifying each of the variables in Stoke's equation at the input to the settler. Of these variables, the liquor density, $\rho_l$, and viscosity, $\mu$, could be calculated from the outputs of the slaker/causticizer model. The density of the mud solids could be obtained from handbooks. However, there appears to be no way to calculate lime mud particle size from the existing slaker/causticizer outputs. Furthermore, nothing appears to be available in the
literature for predicting mud particle size per se. Thus, some method will have to be devised for calculating the mud particle size based upon empirical data.
SOLIDS SETTLING MODEL

The settling model can be derived using indirect methods of determining lime mud settling velocity. Several authors have dealt with the problem of determining the effects of different variables in slaking, causticizing, and calcining on the mud settling velocity (References 6,8,9). Figures 4 through 8 show the results of experiments conducted by K. Kinzner. Figure 4 shows the effect of causticizing time and temperature on the lime mud settling velocity. It is evident from Figure 4 that the longer causticizing times result in a slower settling mud, probably because the added agitation decreases the flocculated particle size. That increased amounts of agitation in causticizing are detrimental to mud settling has been established by Dorr and Bull (Reference 9). The top graph of Figure 5 shows the effect of over-liming, too much lime being detrimental to the settling rate. Evidently, over-liming produces fine particles of CaO and Ca(OH)\(_2\) in the causticized liquor which do not settle out readily. The bottom graph of Figure 5 shows the effect of changing the proportion of the green liquor flow being added to the slaker (the remainder being added directly to the classifier). The proportion added to the slaker is rarely below 40% in practice. Figure 6 shows the effect of the green liquor concentration (entering the slaking/causticizing reaction) on the mud settling velocity. The probable cause of this result was mentioned previously.

Calcining probably has a substantial effect on the size and structure of the lime mud particle. The effect of the CaO particle
FIGURE 4

EFFECT OF CAUSTICIZING TIME AND TEMPERATURE ON LIME MUD SETTLING VELOCITY
FIGURE 5

EFFECT OF LIME QUANTITY AND GREEN LIQUOR QUANTITY ON LIME MUD SETTLING VELOCITY
**FIGURE 6**

EFFECT OF GREEN LIQUOR CONCENTRATION ON LIME MUD SETTLING VELOCITY
FIGURE 7

EFFECT OF CALCINATION TIME ON LIME MUD SETTLING VELOCITY
FIGURE 8

EFFECT OF CALCINATION TEMPERATURE 
ON LIME MUD SETTLING VELOCITY
size on the settling rate of CaCO₃ has been established by Olsen and Direnga (Reference 8). In general, the larger the CaO particle entering slaking/causticizing, the faster the settling of the CaCO₃. The results shown in Figures 7 and 8 indicate agreement with the results of Olsen and Direnga. That is, that calcining time and temperature affect the CaO particle size which in turn affects the CaCO₃ particle size and its settling characteristics. The larger calcining temperature and calcining time result in a larger, more dense, CaO particle, as indicated by Figures 7 and 8.

Figure 9 shows the effect of lime mud solids concentration on the settling velocity of a typical lime mud (10). Although the graph of Figure 9 does not show it, the effect of changes in lime mud particle size would be a family of curves approximately parallel to the one shown. This would have to be established by further settling tests.

Figure 10 illustrates the cross-section of a typical lime mud settler used in the recovery system along with its steady-state concentration profile. Normally, the concentration of solids in the feed mixture will be quite high (about 400 grams/liter of CaCO₃, or about 15% by volume). In that case, the settling zone (zone 2) will be very narrow, and zone 3 will be very wide. If the mud particle settling velocity decreases, or if the underflow decreases, the settling zone will back up into the clarification zone and eventually some of the mud particles will be withdrawn with the overflow. This is the type of action we wish to describe in the dynamic model.
CONCENTRATION EXPRESSED AS

\[ \text{Na}_2\text{O} \]

FIGURE 9

CONCENTRATION VERSUS SETTLING RATE
FOR TYPICAL LIME MUD SLURRY
FIGURE 10

DIAGRAM OF A CONTINUOUS CLARIFIER/THICKENER
AND CORRESPONDING TYPICAL CONCENTRATION PROFILE
The feed mixture enters the settler several feet below the surface of the clarification zone. In typical modern industrial recovery systems, the settler units double as storage units for the overflow liquid so that normally the clarification zone (zone 4) is very wide. The feed mixture enters at the level of zone 3 where it disperses horizontally, and the solids begin to settle. (The horizontal concentration profile is of no interest to us.) The clarified liquid is drawn off at the overflow, while the mud slurry is withdrawn at the underflow at about 35% solids.

The vertical velocity of the mud particles relative to the settler wall is the resultant of three vertical components:

\[ v_s = u_s - u_w + v_b \] (11)

where

- \( u_s \) = Vertical settling velocity relative to wall (ft/hr)
- \( u_w \) = Upward velocity of the liquid caused by the displacement of the downward moving solids (ft/hr)
- \( v_b \) = Upward (or downward) velocity of the entire bulk volume (ft/hr)
- \( v_s \) = Vertical settling velocity relative to wall (ft/hr)

Actually there are two expressions for \( v_s \):

\[ v_{s1} = u_s - u_w - v_{bl} \] (12a)
\[ v_{s2} = u_s - u_w - v_{b2} \] (12b)

where \( v_{s1} \) is the velocity of the particles in the zone above the feed inlet, and \( v_{s2} \) is the velocity below the feed inlet. \( v_{bl} \) and
and \( v_{b2} \) are created by the overflow and underflow respectively, and are obtained as follows:

\[
\begin{align*}
    v_{bl} &= q_o / A \\
    v_{b2} &= q_u / A
\end{align*}
\]

where

\[
\begin{align*}
    A &= \text{Cross-sectional area of the settler (ft}^2) \\
    q_o &= \text{Overflow flow rate (ft}^3/\text{hr}) \\
    q_u &= \text{Underflow flow rate (ft}^3/\text{hr}) \\
    v_{bl} &= \text{Upward velocity of the entire bulk volume in the zone above the feed inlet (ft/hr)} \\
    v_{b2} &= \text{Downward velocity of the entire bulk volume in the zones below the feed inlet (ft/hr)}
\end{align*}
\]

The above discussion assumes no velocity gradients in the horizontal plane which, of course, is not completely accurate. But this assumption does not appear to be detrimental to the ultimate goal of achieving a reasonable vertical concentration profile. An approximate vertical bulk velocity profile for a typical settler is shown in Figure 11. The increase in velocity in zone 1 results because the area of the settler decreases. (The bottom slopes toward the center.)

\[
u_n = u_s - u_w
\]

In the free settling zone, \( u_w \) is zero for all practical purposes. However, it becomes more and more significant in the two compression zones. \( u_s \) would be given by Equation (10) or modifications thereof. However, because data are not available for the variables in
FIGURE 11

APPROXIMATE VERTICAL BULK VELOCITY PROFILE FOR CONTINUOUS SETTLING
Equation (10), we must rely on empirical data given by settling tests. Thus, by using data such as given in Figures 4 through 8, one can establish a regression equation for \( u_n \):

\[
u_n = f(t_c, T_c, L, G, G_c, t_K, T_K)
\]

(15)

where

- \( G \) = Green liquor to slaker (%)
- \( G_c \) = Green liquor concentration (lb/ft\(^3\))
- \( L \) = Lime quantity (%)
- \( T_c \) = Causticizing temperature (°F)
- \( t_c \) = Causticizing time (hrs)
- \( T_K \) = Calcining temperature (°F)
- \( t_K \) = Calcining time (hrs)

In zone 1, the solids are highly compressed, and therefore \( u_n \to 0 \). Hence, one can assume that the vertical velocity is equal to \( v_b \).

In the development of the dynamic model, several assumptions will be made.

1. No horizontal gradients of the variables.
2. No chemical reactions.
3. Uniform temperature (i.e., adiabatic process).
4. The density of the clear liquid and of the dry solids does not change.

Assumptions 2, 3, and 4 raise no particular difficulties. Assumption 1, as mentioned previously, does not appear detrimental to
our goal of achieving an average vertical solids concentration profile with respect to the horizontal space variables. With these assumptions in mind, we can proceed with the model derivation.

If one considers a small stationary volume within the settler, a mass conservation equation can be written about this small volume with respect to the solids concentration:

$$\frac{\partial C_{lm}}{\partial t} + \frac{\partial (C_{lm} v_s)}{\partial z} = 0 \quad (16)$$

where

$$C_{lm} = \text{Concentration of mud solids (lb/ft}^3\text{)}$$

$$v_s = u_n + v_b \text{ (ft/hr)}$$

Expanding the second term of (16) and substituting for $v_s$, we have:

$$\frac{\partial C_{lm}}{\partial t} = - C_{lm} \frac{\partial v_s}{\partial z} - v_s \frac{\partial C_{lm}}{\partial z}$$

$$= - C_{lm} \frac{\partial (u_n + v_b)}{\partial z} - (u_n + v_b) \frac{\partial C_{lm}}{\partial z}$$

or

$$\frac{\partial C_{lm}}{\partial t} = - C_{lm} \frac{\partial u_n}{\partial z} - C_{lm} \frac{\partial v_b}{\partial z} - (u_n + v_b) \frac{\partial C_{lm}}{\partial z} \quad (17)$$

By using our knowledge of what happens physically in each of the settling zones, we can modify Equation (17) appropriately to fit each of the zones of settling. In zone 4, the clarification zone, the solids concentration should be zero everywhere, so that Equation (17) vanishes identically. In the free settling zone, the gradient of $u_n$ with respect to $z$ is zero. That is, $u_n$ is a
constant in free settling and is approximately determined by Stoke's law (11). Thus in zone 3 we have

$$\frac{\partial C_{lm}}{\partial t} = -(u_n + v_b) \frac{\partial C_{lm}}{\partial z} - C_{lm} \frac{\partial v_b}{\partial z} + W_{\text{CaCO}_3I}$$

(17a)

where

$$W_{\text{CaCO}_3I} = \text{Input flow rate of solids at the feed (lb/ft}^3\text{-hr)}$$

Actually, there will be two equations representing the dynamics occurring in zone 3: One for the volume above the level of the inlet; and another for the volume below the level of the inlet. The sign of the bulk velocity must be appropriate for each part. $W_{\text{CaCO}_3I}$ is zero for the upper part. As stated previously, the concentration of solids above the inlet is normally zero. But when, under dynamic conditions, the width of the zone increases so that the sum of the widths of the compression zones and the settling zone is above the level of the inlet, it will be necessary to "switch on" the equation for the upper part, using the appropriate boundary conditions and initial conditions.

In the compression zone, the solid particles begin to interfere with one another, and there is a definite dependence of settling velocity $u_n$ on solids concentration $C_{lm}$. Moreover, the concentration is dependent upon the level $z$ in the compression zone. This phenomenon can be described by expanding the partial derivative in the first term on the right hand side in Equation (17) using the chain rule:
\[
\frac{\partial u_n(c_{lm}(z))}{\partial z} = \left[ \frac{\partial u_n}{\partial c_{lm}} \right] \frac{\partial c_{lm}}{\partial z}
\]

Furthermore, as Figure 11 indicates, the bulk velocity gradient with respect to \( z \) should be zero. Therefore in zone 2 we have

\[
\frac{\partial c_{lm}}{\partial t} = - \left( u_n + v_b + C_{lm} \frac{\partial u_n}{\partial c_{lm}} \right) \frac{\partial c_{lm}}{\partial z} \quad (17b)
\]

In the rake action compression zone, as mentioned previously, \( u_n \) is approximately zero, and therefore only the bulk velocity is significant. Thus in zone 1 we have

\[
\frac{\partial c_{lm}}{\partial t} = - v_b \frac{\partial c_{lm}}{\partial z} - C_{lm} \frac{\partial v_b}{\partial z} \quad (17c)
\]

We note that Equations 17a through 17c are a set of first order partial differential equations with varying coefficients. However, these coefficients are known functions of the causticizing and calcining conditions, of the incoming and outgoing flow rates, and of the physical dimensions of the settling tank. Therefore, the equations may be solved by applying the appropriate boundary and initial conditions, and they will yield a dynamic vertical concentration profile in the settler. A steady-state profile can be attained by setting the \( \frac{\partial c_{lm}}{\partial t} \) term equal to zero in each of the Equations (17) and solving. The dynamic volume balance for the settler is:

\[
\frac{\partial Q}{\partial t} = q_i - q_o - q_u \quad (18)
\]
where

\[ Q = \text{Volumetric accumulation of liquid plus solids (ft}^3\text{)} \]

\[ q_i = \text{Input flow rate at the feed (ft}^3/\text{hr)} \]

\[ q_o = \text{Overflow flow rate (ft}^3/\text{hr)} \]

\[ q_u = \text{Underflow flow rate (ft}^3/\text{hr)} \]

The dynamic mass for solids in the settler is given by:

\[ \frac{dm_s}{dt} = q_i C_i = q_u C_u - q_o C_o \tag{19} \]

where

\[ C_i = \text{Input solids concentration (lb/ft}^3\text{)} \]

\[ C_o = \text{Overflow solids concentration (lb/ft}^3\text{)} \]

\[ C_u = \text{Underflow solids concentration (lb/ft}^3\text{)} \]

\[ m_s = \text{Total mass of solids in the settler (lb)} \]

The liquid concentration in the underflow can be obtained by using the relation:

\[ \frac{C_u}{\rho_s} + \frac{L_u}{\rho_1} = 1 \]

or

\[ L_u = \rho_1(1 - \frac{C_u}{\rho_s}) \tag{20} \]

where

\[ L_u = \text{Underflow liquid concentration (lb/ft}^3\text{)} \]

\[ \rho_s \text{ and } \rho_1 \text{ are defined in Equation (10).} \]

A similar expression can be obtained for the liquid concentration of the overflow.
FURTHER COMMENTS ON LIME MUD PARTICLE SIZE

It was previously implied that lime mud particle size is an important parameter, not only in white liquor clarifying and mud washing, but also in mud filtering and dewatering prior to calcining. It is not within the scope of this Section to dynamically model the mud vacuum filtering process. However, the important characteristic of the lime mud in vacuum filtering and dewatering is the particle size. The previous implication was that it would be very difficult to obtain data on lime mud particle size without extensive and tedious testing or the use of very specialized instrumentation. However, one can infer a particle size from the data obtained in settling tests (where results would be similar to those shown in Figures 4 through 8) and from Stoke's law (Equation 10). Rewriting Equation (10) we have

\[
\bar{D}^2 = \frac{u_n}{Kg(\bar{\rho}_s - \rho_1)}
\]

or

\[
\bar{D} = \sqrt{\frac{u_n^2}{Kg(\bar{\rho}_s - \rho_1)}}
\]

where

- \(\bar{D}\) = An approximate value for the mean diameter of the mud particles (ft)
- \(u_n\) = Settling velocity obtained from regression equation (Equation 15) (ft/hr)
- \(\bar{\rho}_s\) = An approximate value for the density of dry CaCO\(_3\) (lb/ft\(^3\))

Thus, one could use \(\bar{D}\) as a time varying parameter in the vacuum filtering and dewatering equations.
REFERENCES CITED


SECTION VIII

DETERMINATION OF A MATHEMATICAL MODEL
FOR A ROTARY LIME KILN

INTRODUCTION

Although the importance of a lime kiln in the recausticizing process has been recognized, the literature on the behavior of a rotary lime kiln is scare. While rotary lime kilns have been ignored, several studies on cement kilns have been reported [1, 2, 3]. The steady-state behavior of a cement kiln has been simulated [1, 2] using a set of ordinary differential equations. This model (particularly some numerical values) appears empirical to a large extent; however, no systematic method is presented for the determination of the parameter values. This empirical model has also been used for determining the moisture content of the material [2] which is feed into a kiln so as to minimize fuel costs per ton of production. It is noted that the model of a cement kiln can be adopted for the representation of a lime kiln, since the same processes of evaporation, calcination, combustion and heat transfer take place in both types of kiln.

Some specific aspects of a rotary kilns, such as heat transfer, have been investigated [4, 5, 6, 7 and 8]. In particular, the dependence of the rate of calcination upon the mass and heat transfer rates and the rate of nucleation has been studied extensively [6]. The combustion has been investigated by comparing the use of various fuels such as coal, gas and oil [3]; also a simplified model for a rotary cement kiln was introduced [3].
The purpose here is to develop a systematic method to determine a mathematical model that describes the behavior of a rotary lime kiln. The form of the mathematical equations are obtained on the basis of physical laws. The unknown parameters are then determined so that a least-squares fit is obtained for the measured data.

The purpose of the lime kiln is to convert the lime mud (CaCO$_3$ + H$_2$O) to lime (CaO), in such a manner as to give a lime product with the best physical and chemical qualities for the recausticizing process. The reburnt lime from the kiln should ideally be porous and completely calcined so that it will slake easily and so that the lime mud will settle rapidly. An ideal reburnt lime is produced when the dried lime mud is heated to 1550-1600°F and held there until all carbon dioxide (CO$_2$) is evolved. If the temperature is held too high, some of the lime becomes non-porous and will not slake easily. If the temperature is too low and/or the lime has not burnt long enough, some lime may not be calcined and consequently will not slake. The reburning of lime at 1550°-1600°F until a complete calcination occurs would require a very large rotary kiln, because the calcination would proceed very slowly; as a result, a large amount of material would be held in the kiln. Therefore, a large kiln produces, in general, better lime than a smaller kiln providing that both kilns are properly operated; however, the former is more expensive.

In a typical rotary kiln, the ratio of the length to the inner diameter is about 30:1. The inner diameter is determined by the rate at which material is processed. The time which a solid particle needs to traverse the length of the kiln is usually
called the residence time. A typical value of the residence time is 1.5-2 hours for a rotary lime kiln.
The mathematical form of the equations that describe the behavior of a rotary lime kiln is derived on the basis of the conservation of mass and heat energy. The equations for the mass and heat energy balances are written at a point \((t, l)\) of the kiln specified at time \(t\) and the distance \(l\) (in feet) measured from the point where lime mud enters the kiln. The equations are obtained under the following assumptions:

(i) The specific heat coefficients, the latent heat and the amount of heat generated or needed in reactions are constant.

(ii) The fuel used is methane \((CH_4)\) and the combustion is assumed to be complete.

(iii) Possible impurities and inert compounds are omitted in writing the expressions for the material and energy balances.

(iv) Possible solid particles in the gas flow are ignored.

(v) The residence time of the burden mass in the kiln is inversely proportional to the angular spin and proportional to the length of the kiln.

(vi) The burden mass held in the kiln at any time is directly proportional to the flow rate of the burden mass.

A detailed derivation of the dynamical equations of a kiln is presented below.

The dynamical equations describing the behavior of a kiln can be represented in a concise form as:
\[ \frac{\partial q(t,t;\alpha)}{\partial t} = A_0(\alpha) \frac{\partial q(t,t;\alpha)}{\partial t} + F_1(q,t,t;\alpha) \quad (1) \]

\[ F_2(q;\alpha) = 0 \quad (2) \]

where \( q = \text{col} \left[ X_{CaO_3}, X_{CaO}, X_{w}, Y_{O_2}, Y_{w}, Y_{CO_2}, T_s, T_g \right] \) signifies the distributed state of the system defined on \((0,L) \times (0,t_f)\). \( \alpha \) is a parameter vector defined by \( \alpha = \text{col} \left[ \alpha^1, \ldots, \alpha^s \right] \) with \( s \) a positive integer.

The mathematical time-invariant model for the steady-state operation of a kiln is obtained by setting \( \frac{\partial q}{\partial t} = 0 \) in Equation (1). The resulting equations are:

\[ A_0(\alpha) \frac{\partial q(t;\alpha)}{\partial t} + F_1(q,t;\alpha) = 0 \quad (3) \]

\[ F_2(q;\alpha) = 0 \quad (2) \]

Hence, the mathematical form that describes the dynamical behavior of the kiln is specified by Equations (1) and (2), and under steady-state conditions by Equations (2) and (3). These equations contain an unknown parameter vector \( \alpha \), which is to be computed on the basis of available measurements.

DETERMINATION OF THE SYSTEM PARAMETERS

The parameter vector is computed by constructing algorithms to minimize an error measure on the basis of a deterministic or
stochastic gradient depending upon the accuracy of the measurements (noise excluded or included).

(a) Exact Measurements

The steady-state equations for the kiln are given by Equations (2) and (3). The exact measurement is specified by

\[ z(t_i) = D(t_i) q(t_i), \quad i, \ldots, N \]  

where \( D \) is an 8th order diagonal matrix and \( t_i \) specifies one of the \( N \) measurement points (\( N \) is a positive integer).

An error measure is chosen as follows:

\[ E(a) = \sum_{i=1}^{N} \left\| z(t_i) - D(t_i) q(t_i, a) \right\|_w^2 \]  

where \( q \) is a solution of the steady-state equations for a particular value of \( a \). \( \| \cdot \|_w \) is the Euclidian norm, i.e. \( \| z \|_w^2 = z' w z \). The problem is to find a value \( a = a^* \) such that \( E(a) \) is minimal.

A possible procedure is to choose initially a value of \( a = a^0 \), and iterate on the value of \( a^i \), \( i = 0, 1, \ldots \) using a gradient technique so as to attain a minimum of the error criterion (5).

The computations are performed as follows. The initial value \( a^0 \) is obtained, for example, from literature on the simulation of rotary cement kilns [1,2]. Equations (2) and (3) are solved digitally, and \( E(a^i) \) in the \( i^{\text{th}} \) iteration is calculated. Then, a grid search for a new value \( a^{i+1} \) of the parameter vector is performed. An approximate gradient \( \Delta E/\Delta a^i \) is computed by varying each component of \( a^i \) by an amount \( \Delta a^i \) and calculating the corresponding change \( \Delta E(a^i) \) in \( E(a^i) \). Hence, an approximate gradient of \( E(a^i) \) can be determined:
\[
\varepsilon_j^i = \frac{E(\alpha_i + \Delta \alpha_j^i) - E(\alpha_i^i)}{\Delta \alpha_j^i}; \quad j=1,\ldots,
\]  

(6)

where \(\varepsilon_j^i\) is the \(j^{th}\) component of the approximate gradient vector. Then, a new value \(\alpha_i^i+1\) is chosen by taking a small step \(p\) in the negative gradient direction, which decreases the value of the error criterion.

\[
\alpha_i^i+1 = \alpha_i^i - p\varepsilon_i^i
\]

(7)

One proceeds in this direction by increasing \(p\) as long as \(E(\alpha_p^i)\) decreases. In this manner, the approximate minimum of \(E(\alpha_p^i)\) along the line given by Equation (7) is found by performing a cubic curve fit to the last four values of \(E(\alpha_p^i)\). The procedure is repeated until the change in \(E(\alpha)\) is no longer significant.

This iterative procedure is now summarized: (i) Choose \(\alpha^o = \alpha_{\text{init}}\) and compute \(E(\alpha^o)\). (ii) Compute gradient \(g_i^1\). (iii) Proceed in this direction until \(E(\alpha_i^1 - pg_i^1)\) is minimal; set \(E(\alpha_i^1+1) = E(\alpha_i^1 - p\varepsilon_i^1)\). (iv) If \(|E(\alpha_i^1+1) - E(\alpha_i^1)| < \zeta\), where \(\zeta\) is a small chosen number, accept the numerical values and stop; otherwise, repeat from (ii) on.

The iterations are repeated until the error criterion \(E(\alpha_i^1)\) cannot be decreased anymore. The corresponding value of the unknown parameter vector furnishes a local minimum of \(E(\alpha)\). It is accepted as the (locally) best parameter vector for the mathematical model.

(b) Noise-corrupted Measurements

Suppose that the measurements are corrupted by noise. Thus, Equation (4) is replaced by
\[ z(t_i) = D(t_i) \cdot q(t_i) + \eta(t_i), \quad i = 1, \ldots, N \quad (8) \]

where \( q(t_i) \) is the state corresponding to the true value of \( a \). \( \eta(t_i) \) signifies measurement error (noise). These noise terms are uncorrelated with one another and with state variables; moreover, they possess zero mean and finite variance. It is assumed that \( N \) measurements, Equation (8), are attained sequentially. The \( n^{th} \) set of measurement data is denoted by a subscript \( n \), e.g., \( z_n(t_i) \), \( \eta_n(t_i) \). In order to construct a sequential algorithm for the identification of the best parameter \( a^* \), an error criterion is defined as

\[ E(a_n) = \sum_{i=1}^{N} \| z_n(t_i) - D(t_i) \cdot q(t_i; a_n) \|_w^2 \quad (9) \]

where \( n = 0, 1, \ldots \)

The \( k^{th} \) component of \( a_n \) is denoted by \( a_{n}^k \), and the corresponding unit vector in the \( s \)-dimensional parametric space by \( e^k \). The stochastic approximation algorithm is then specified by

\[ a_{n+1} = a_n - \frac{a_n}{b_n} G_n, \quad n = 1, 2, \ldots \quad (10) \]

In Equation (10), \( G_n \) represent a stochastic gradient vector whose \( k^{th} \) component is determined by

\[ G_n^k = \frac{1}{2 \gamma} \left[ E(a_n^1, \ldots, a_n^k + e^k \gamma, \ldots, a_n^s) - E(a_n^1, \ldots, a_n^k \right. \\
\left. - e^k \gamma, \ldots, a_n^s) \right], \quad k = 1, \ldots, s \quad (11) \]

where \( \gamma \) is a scale factor chosen such that the parameter values are admissible. The sequence \( \{a_n/b_n\} \) consists of positive real
numbers such that (i) \( a_n/b_n \rightarrow 0 \) as \( n \rightarrow \infty \); (ii) \( \sum_{n=1}^{\infty} (a_n/b_n) = \infty \); (iii) \( \sum_{n=1}^{\infty} (a_n/b_n)^2 < \infty \).

It is noted that properties (i), (ii) and (iii) are satisfied for example by the sequence \( \{1/n\} \).

It can be shown that Algorithm (10) converges in the mean square sense to the true parameter value \( \alpha^* \), if the following assumptions hold: (i) \( \eta_n(\lambda_i) \) for each \( i=1, \ldots, N \) and each \( n = 1, 2, \ldots \) is uncorrelated with one another and with the state variables of the system, and satisfies \( P[|\eta_n(\lambda_i)| \leq M] = 1 \), where \( P[\cdot] \) signifies the probability and \( M \) is a positive constant. (ii) If \( \alpha_n^k - \alpha^*_k > 0 \), the \( E[G^k_n | \alpha^k_n] > 0 \), where \( [\cdot] \) denotes the conditional expectation. Also the expressions obtained by reversing the inequality signs in both expressions must hold. (iii) If \( \beta_n = \alpha_n - \alpha^* \), then positive real constant \( K_0 \) and \( K_1 \) exist such that for all \( n \), \( K_1 \leq K_0, K_1 \| \beta_n \| \leq E[|G_n^k| | \alpha^k_n] \| \leq K_0 \| \beta_n \| \). (iv) If \( \overline{G}_n \) indicates the value of \( G_n \) in Equation (11) and (9) in the absence of the noise, then it is required that \( E[G_n^k | \alpha^k_n] = \overline{G}_n \) for unbiased estimates.

It is noted that condition (i) implies that the absolute value of the noise terms is not "too large" in the average. Condition (ii) requires that the error criterion in Equation (9) is strictly convex and unimodel with respect to \( \alpha \). Condition (iii) assures that some correction takes place when \( \alpha_n \) is far from \( \alpha^* \); and that a small correction is performed (without overshooting) when \( \alpha_n \) is close to \( \alpha^* \).

Conditions (i) through (iv) guarantee the convergence of Algorithm (10) in the mean square sense.
In the applications, it is naturally difficult to check whether or not the aforementioned conditions are fulfilled. Indeed, this aspect will not be studied here. On the other hand, one should still recognize that these requirements provide engineers with some guidelines in understanding the behavior of the algorithm in a complex problem.

APPLICATION TO A SPECIFIC KILN

The rotary kiln studied is 250' long and has an outside diameter of 9' 2 1/2" when it is cold, and weighs about 560 tons. The kiln slopes toward the hot end at 1/2" per lineal foot. It is supported at four places, where it turns on trunions at rates of 1.5, 1.125, 0.75, and 0.5625 rpm normally and at 0.1 rpm, when the kiln is on auxiliary drive.

The interior of the kiln can be divided into three sections: (i) chain section, (ii) preheating section, and (iii) combustion zone. The drying zone extends from 0' to 34' and is lined with castable refractory to a 4 1/2" thickness. The chains are hung for 6' to 32'. The preheating section (34' to 170') and the combustion zone (170' to 250) are lined with a 6" thickness of alumina brick. (Figure 2)

The points at which the measurements in the kiln are performed are shown in Figure 2. The measurements obtained from the aforementioned kiln are shown in Table I.

The components of the burden mass are measured at points $P_1, P_2, P_3$, and $P_5$ by taking a sample and having it analyzed. The gas components are measured by taking a sample and having it analyzed. The flow rate is measured by using a pitot tube.
FIGURE 1. MEASUREMENT POINTS ALONG KILN.

FIGURE 2. SAMPLING TECHNIQUE AT $p_2$ & $p_3$
<table>
<thead>
<tr>
<th>Measurement</th>
<th>(P₁,1)</th>
<th>(P₂,2)</th>
<th>(P₃,3)</th>
<th>(P₄,4)</th>
<th>(P₅,5)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Point(P₁,1)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>λ₁ (ft)</td>
<td>6</td>
<td>22</td>
<td>35</td>
<td>108.5</td>
<td>250</td>
</tr>
<tr>
<td>qₖ(λ₁)</td>
<td>q₁, j=1,...,8, q₁,q₂,q₃,q₇</td>
<td>q₁,q₂,q₃,q₇,q₈</td>
<td>q₈</td>
<td>qₖ, j=1,...,8</td>
<td></td>
</tr>
</tbody>
</table>

* Distance from the feed-end of the kiln

\[ q₁ = X_{CaCO₃}, \quad q₂ = X_{CaO}, \quad q₃ = X_w, \quad q₄ = Y_{O₂}, \quad q₅ = Y_w \]

\[ q₆ = Y_{CO₂}, \quad q₇ = T_s, \quad q₈ = T_g \]
The measurement of the burden temperature at $P_5$ is sometimes quite inaccurate due to dusting. The gas temperature at $P_5$ is an estimated value; similarly, the amount of water vapor at $P_1$. Also, the flame length is difficult to approximate, because the viewing port of this particular kiln is low and on the right side of the firing hood so that the view is obscured by the burden mass. The actual rate of lime feed into the kiln cannot be measured directly; only the flow rate to the dewatering centrifuge is obtained.

Typical operating conditions for the kiln described are given in Table II.

SIMULATION RESULTS FOR THE IDENTIFICATIONS

The mathematical model of the aforementioned kiln was determined by computing the parameter values. The 13 parameters computed are specified in Table III. These values provide a local minimum for the error criterion (5).

The simulated profiles of the burden composition, the gas and burden temperatures associated with the optimal parameter value $\alpha^*$ are shown in Figures 3 and 4. The procedure converged to a local minimum value of $E(\alpha)$ in 16 iterations using 4 1/2 minutes of computer time and 25k of memory on a CDC 6500 computer. It is noted, however, that the program was not "polished"; consequently, the computer time and memory requirements are amenable to considerable improvements, if it is necessary.
<table>
<thead>
<tr>
<th>Variable</th>
<th>Meas. Locations</th>
<th>Measured Values</th>
</tr>
</thead>
<tbody>
<tr>
<td>$T_s = q_7$</td>
<td>$P_1, P_2, P_3$</td>
<td>115, 160, 180, 1100°F, respectively</td>
</tr>
<tr>
<td>$T_g = q_8$</td>
<td>$P_1, P_3, P_4$</td>
<td>510, 1100, 1400°F, respectively</td>
</tr>
<tr>
<td>$C_{ps} = q_9$</td>
<td></td>
<td>0.26 Btu/lb.-°F</td>
</tr>
<tr>
<td>$C_{pg} = q_{10}$</td>
<td></td>
<td>0.28 Btu/lb.-°F</td>
</tr>
<tr>
<td>$W_b = q_{11}$</td>
<td></td>
<td>$5.0 \times 10^3$ lb/hr</td>
</tr>
<tr>
<td>$W_{gN} = q_{12}$</td>
<td></td>
<td>$27 \times 10^3$ lb/hr</td>
</tr>
<tr>
<td>$X_w = q_{13}$</td>
<td>$P_1, P_2, P_3$</td>
<td>35, 16, 3% (wet basis), respectively</td>
</tr>
<tr>
<td>$X_{O_2} = q_{14}$</td>
<td>$P_1$</td>
<td>6.8-7.2% (dry basis)</td>
</tr>
<tr>
<td>$X_{CO_2} = q_{15}$</td>
<td>$P_1$</td>
<td>14% (dry basis)</td>
</tr>
<tr>
<td>$X_{CaO} = q_{16}$</td>
<td>$P_5$</td>
<td>89.6%</td>
</tr>
<tr>
<td>$T_g = q_{17}$</td>
<td>$P_5$</td>
<td>750°F (estimated)</td>
</tr>
<tr>
<td>$\Theta = q_{18}$</td>
<td></td>
<td>1 1/2-2 hr</td>
</tr>
</tbody>
</table>

Fuel mass flow rate 1.3×10^3 lb/hr

* A.S.T.M. "rapid" sugar test was used to determine % active lime.
<table>
<thead>
<tr>
<th>Parameter</th>
<th>$a_1=f_1$</th>
<th>$a_2=f_2$</th>
<th>$a_3=f_3$</th>
<th>$a_7=e_s$</th>
<th>$a_8=e_s$</th>
<th>$a_9=e_w$</th>
<th>$a_{10}=A_w$</th>
<th>$a_{11}=\Delta E_w$</th>
<th>$a_{12}=A_c$</th>
<th>$a_{13}=\Delta E_c$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Final Value</td>
<td>8.77*</td>
<td>97.10*</td>
<td>44.11*</td>
<td>0.073</td>
<td>0.790</td>
<td>0.932</td>
<td>2.21 \times 10^7</td>
<td>21,300**</td>
<td>1.26 \times 10^{27}</td>
<td>251,000**</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Parameter</th>
<th>$a_4=f_1$</th>
<th>$a_5=f_2$</th>
<th>$a_6=f_3$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Value</td>
<td>3.86*</td>
<td>3.96*</td>
<td>39.11*</td>
</tr>
</tbody>
</table>

* Btu/hr-ft$^2$-°F
** Btu/lb-mole
° Hr$^{-1}$
FIGURE 3. BURDEN PROFILE OF ROTARY LIME KILN.
FIGURE 4. TEMPERATURE PROFILE OF ROTARY LIME KILN.

Measured values of gas temperature
Measured values of burden temperature

Distance, $L$, from feed end of kiln, in feet

Gas and burden temperatures in degrees Rankine
LINEARIZED MODEL FOR KILN

Equations (1) and (2) describing the dynamic behavior of the rotary lime kiln may be written in the component form as

\[ \frac{\partial q_i(t)}{\partial t} = \sum_{j=1}^{9} \left( A_0(q,u,t) \right)_{ij} \frac{\partial q_j(t)}{\partial t} F_1^i(q,u,t) \]  

(12)

where \( i = 1, 2, \ldots, 9 \) and \( (A_0(q,u,t))_{ij} \) is the \( ij \)th element of \( A_0(q,u,t) \)

\[ F_2^i(q) = 0 \quad i = 1, 2, \ldots, 20. \]  

(13)

The linearization of Equations (12 and 13), omitting functional dependence, results in

\[ \frac{\partial q_i(t)}{\partial t} = \sum_{j=1}^{9} (A_0)_{ij} \frac{\partial q_j(t)}{\partial t} q + \sum_{j=1}^{9} \left\{ \sum_{k=1}^{9} \left[ \frac{\partial A_0}{\partial q_k} \right]_{ij} \frac{\partial q_j(t)}{\partial t} + \frac{\partial F_1^1}{\partial T_w} \frac{\partial q_j(t)}{\partial t} \right\} \]  

(14)

where \( q \) and \( u \) represent small perturbations about the nominal solution. \( T_w \) is the inside kiln wall temperature.

Defining,

\[ (A_\lambda)_{ij} = - (A_0)_{ij} \]  

(15)
\[
(Aq)_{ik} = \sum_{j=1}^{9} \left( \frac{\partial A_0}{\partial q_j} \right)_{ij} \frac{\partial q_j}{\partial t} + \left( \frac{\partial A_0}{\partial T_w} \right)_{ij} \frac{\partial T_w}{\partial q_k} \frac{\partial q_k}{\partial t} + \frac{\partial F_1}{\partial q_k} + \frac{\partial F_1}{\partial T_w} \frac{\partial T_w}{\partial q_k}
\]

and
\[
(Au)_{ik} = \sum_{j=1}^{9} \left( \frac{\partial A_0}{\partial u_j} \right)_{ij} \frac{\partial q_j}{\partial t} + \frac{\partial F_1}{\partial u_k}
\]

then Equation (14) can be rewritten in matrix notation as
\[
\frac{d\hat{q}(t,t)}{dt} + A_q(\hat{q},\hat{u},\hat{\xi}) \frac{d\hat{q}(t,t)}{dt} = A_q(\hat{q},\hat{u},\hat{\xi},\frac{\partial \hat{q}}{\partial \xi}) \hat{q}(\xi,t)
\]
\[
+ A_u(\hat{q},\hat{u},\hat{\xi},\frac{\partial \hat{q}}{\partial \xi}) \hat{u}(t)
\]

and Equation (13) becomes
\[
F_2(q) = 0
\]

The linearized model of the rotary lime kiln will be used to determine a control, U(t), which optimizes the performance of the linearized model in some sense. Such a design will take care of minor upsets and return the distributed state of the lime kiln to the nominal trajectory (e.g., steady-state) in such a manner that a well defined performance index is minimal.
### LIST OF SYMBOLS USED

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>Heat transfer area (sq. ft./ft.)</td>
</tr>
<tr>
<td>B</td>
<td>Calcinable mass/unit length (lb./ft.)</td>
</tr>
<tr>
<td>( C_{pg} )</td>
<td>Specific heat of gas (B.T.U./lb.-°R)</td>
</tr>
<tr>
<td>( C_{ps} )</td>
<td>Specific heat of burden (B.T.U./lb.-°R)</td>
</tr>
<tr>
<td>( \varepsilon )</td>
<td>Emissivity</td>
</tr>
<tr>
<td>( \Delta E )</td>
<td>Activation energy (B.T.U./lb.-mole)</td>
</tr>
<tr>
<td>( f )</td>
<td>Conductive and convective heat transfer coefficient (B.T.U./hr.-sq. ft.-°R)</td>
</tr>
<tr>
<td>( h )</td>
<td>Heat transfer coefficient (B.T.U./hr.-ft.-°R)</td>
</tr>
<tr>
<td>H</td>
<td>Heat of reaction (B.T.U./lb.)</td>
</tr>
<tr>
<td>K</td>
<td>Reaction rate coefficient (hr.(^{-1}))</td>
</tr>
<tr>
<td>L</td>
<td>Length of kiln (ft.)</td>
</tr>
<tr>
<td>M</td>
<td>Molecular weight</td>
</tr>
<tr>
<td>( M_g )</td>
<td>Mass of gas/unit length (lb./ft.)</td>
</tr>
<tr>
<td>( M_s )</td>
<td>Burden mass/unit length (lb/ft.)</td>
</tr>
<tr>
<td>N</td>
<td>Nitrogen mass/unit length (lb./ft.)</td>
</tr>
<tr>
<td>( R_f )</td>
<td>Rate of combustion/unit nitrogen mass (lb/lb.-hr.)</td>
</tr>
<tr>
<td>( R_w )</td>
<td>Rate of evaporation/unit calcinable mass (lb./lb.-hr.)</td>
</tr>
<tr>
<td>( \Theta )</td>
<td>Residence time (hr.)</td>
</tr>
<tr>
<td>( t )</td>
<td>Real time (hr.)</td>
</tr>
<tr>
<td>( T_a )</td>
<td>Ambient temperature (°R)</td>
</tr>
<tr>
<td>( T_g )</td>
<td>Gas temperature (°R)</td>
</tr>
<tr>
<td>( T_s )</td>
<td>Burden temperature (°R)</td>
</tr>
</tbody>
</table>
\[ T_w = \text{Inner wall temperature (°R)} \]
\[ T_{\text{w}}' = \text{Outer wall temperature (°R)} \]
\[ W_b = \text{Calcinarble mass flow rate (lb./hr.)} \]
\[ W_g = \text{Gas mass flow rate (lb./hr.)} \]
\[ W_{gN} = \text{Nitrogen mass flow rate (lb./hr.)} \]
\[ W_s = \text{Burden mass flow rate (lb./hr.)} \]
\[ X_{\text{CaCO}_3} = \text{CaO in form of \text{CaCO}_2/unit calcinarble mass (lb./lb.)} \]
\[ X_{\text{CaO}} = \text{Free CaO/unit calcinarble mass (lb./lb.)} \]
\[ X_w = \text{Water/unit calcinarble mass (lb./lb.)} \]
\[ Y_{O_2} = \text{Oxygen/unit nitrogen mass (lb./lb.)} \]
\[ Y_w = \text{Water vapor/unit nitrogen mass (lb./lb.)} \]
\[ Y_{\text{CO}_2} = \text{Carbon dioxide/unit nitrogen mass (lb./lb.)} \]
\[ Y_f = \text{Fuel/unit nitrogen mass (lb./lb.)} \]
REFERENCES CITED


