

Mill Application of a New Continuous Digester Model

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A new-generation continuous digester model has been developed based on first principles of fundamental material, energy, and momentum balances. The modeling approach considers all of the important physical and chemical phenomena that are pertinent to digester operations: notably, chip size distribution, dynamics of chip column compaction, diffusion and reaction fluxes between entrapped and free liquor, and relative velocity differences between chip column and liquor flows. The model calculates time-dependent behavior of process conditions including but not limited to chip levels, residual EA (effective alkali) density and Kappa (a measure of the extent of reaction) progression through the digester, temperature and dissolved solids profiles, conversion, and blow consistency. The model emulates real operational conditions as closely as possible so that all process decision variables available to an operator are also similar input variables to the model. The model is fast, nearly 300 times faster than real time on a modern PC, which makes it convenient for a variety of applications. High-fidelity simulations of the model can be used for operating condition optimization, controller design improvements, transition policy development, and training. © 2005 American Institute of Chemical Engineers AICHE J, 51: 2489–2494, 2005

Process Description

Continuous digesters are very complex vertical tubular reactors, used in the pulp and paper industry to remove lignin (a three-dimensional organic polymer loosely based on C₉ hydroxy-phenyl structures that holds fibers into wood) from wood chips. An aqueous solution of sodium hydroxide and sodium hydrosulfide, called white liquor, reacts with porous and wet wood chips.

Usually, continuous digesters are separated into multiple reaction and extraction zones to carry out a specific process sequence. Although the chip flow through the zones is always from top to bottom the liquor flow may alternate between cocurrent (with chips) and countercurrent to achieve desired reaction and extraction rates. Depending on the production needs of a pulp mill and on the state of the art of digester design at the time of installation, there may be numerous differences between digesters. However, common to all is the general sequence of transport and reaction processes that govern the overall operation. Because of the complexities of these physical and chemical phenomena and the fact that wood chips are nonuniform and constantly changing as they

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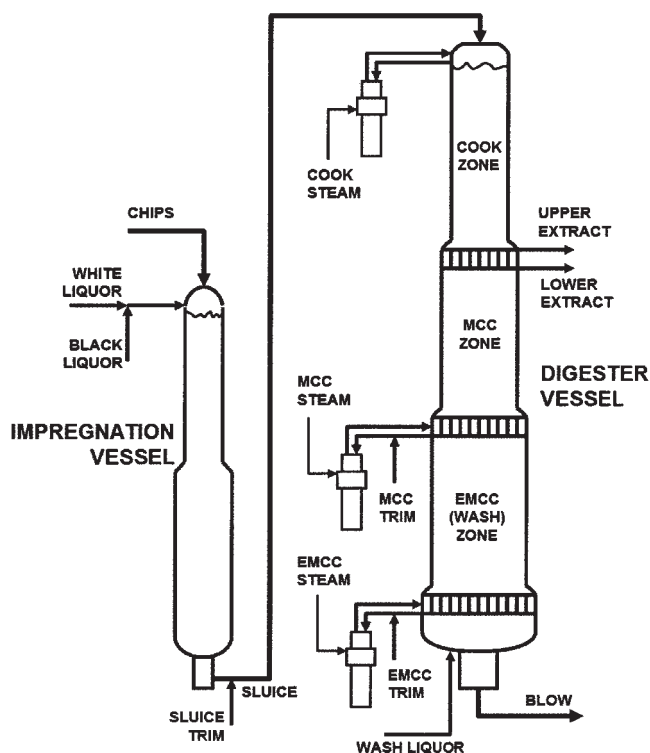


Figure 1. Dual-vessel hydraulic EMCC continuous digester.

travel through the reactor, regulating product quality in a digester is not a trivial task.

The particular digester design for this article is the dual-vessel EMCC (extended modified continuous cooking) arrangement, as shown in Figure 1. A brief description of the process is provided to familiarize the reader with the basics. Detailed descriptions and analyses are available in textbooks and PhD theses on the subject.

Wet chips, steamed to remove air in the pores, are fed into the impregnation vessel together with white liquor. In the impregnation vessel (IV), white liquor penetrates into the chips and equilibrates with initial moisture for about 30 min depending on the production rate. In the IV, both chips and liquor move in the cocurrent downward direction.

From the bottom of the IV, chips are carried into the top section of the digester with hot liquor that brings the mixture to the desired initial reaction temperature. The top section of the digester, referred to as the cook zone, is a cocurrent section where the majority of the reactions take place. Chips react (that is, cook) from inside out as a result of the significant internal pore volume and associated surface area. Therefore, overall reaction rates depend on the concentration levels of entrapped liquor and the diffusion rates from free liquor that replenishes the active ingredient holdup in the pores. Spent liquor saturated with dissolved solids at the end of the cook zone is extracted for chemical recovery elsewhere in the mill. Chips follow into the MCC (modified continuous cooking) and the EMCC zones, now countercurrent to fresh dilute white liquor that continues mild delignification reactions while simultaneously extracting valuable organic solids from the pores of chips.

As packed reactors, digesters are unique in that the solid packing is the main ingredient of the process, which is continuously in motion, nonuniform in size, and undergoes changes through variable compaction with respect to both conversion and differential head pressure. The extent of reaction, defined through the blow-line (exit) Kappa number, is the major performance measurement. The Kappa number is an oxidative test that is an approximate determination of the fractional acid insoluble lignin left in the wood. Other important factors are the yield of the process and the fiber properties of the final product. Although various operating conditions may yield the same Kappa number, important fiber properties such as viscosity and strength may not remain constant at the same final Kappa number because they are also reaction path dependent. Therefore, controlling the performance of a digester is as much a reaction path management problem as it is a stable Kappa number problem.

Features of the New-Generation Model

Continuous digester modeling has gone through significant evolutions starting with the H-factor approximation of Vroom¹ through the fundamental developments by Gustafson,² Butler,³ Christensen,⁴ Wisniewski,⁵ and Michelsen.⁶ Although the transport phenomena-related fundamental issues (such as diffusion and reaction) are modeled with sufficient detail in published models we do not have all of the mechanistic features formulated with sufficient rigor to accurately handle species transition and chip compaction dynamics. Recent efforts by Puig⁷ introduced a mixing parameter approach to approximate transition behavior. The objective of the new fundamental model introduced in this work is to accurately formulate the governing dynamic characteristics of the physical and chemical processes that are needed to track both species and rate transition behavior without severe simplifying assumptions. This central objective is accomplished by incorporating the fundamental contributions of all major previous digester models and by introducing two new components: (1) a unique approach to solid phase modeling and (2) a novel and efficient numerical procedure to solve a large system of model equations.

The main features of the new model can be summarized as:

(1) The solid phase moves in distinct "plugs" downward in the digester, satisfying the experimental evidence of plug-flow behavior. Plug size can be as small as desired for numerical accuracy. For example, about 1200 equal-size solid plugs in a 6-h residence time digester would capture 0.3 min (18 s) flow intervals.

(2) Each plug entering the digester system carries its own distinct set of physical, chemical, and transport properties as model parameters. Thus, there may be multiple simultaneous wood species in the digester at any given time.

(3) Chip size distributions are represented by discrete size mass fraction allocations for chip thickness classifications, similar to industry practice for chip characterization, given that thickness is the controlling dimension for conversion reactions. Usually five to seven size-cut categories are sufficient to represent practical differences between chip thickness variations. Discrete size-cut dimensions are preassigned for practical reasons, yet each plug can have its own designated mass fractions to track chip size variability. Following Gustafson² geometric

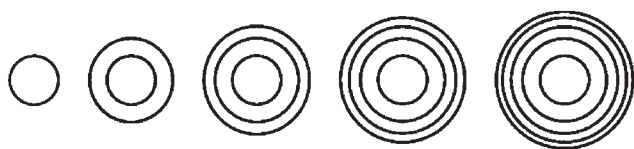


Figure 2. Chip size (thickness) distribution approximation by equivalent volume spheres and spatial discretization of diffusion effects through multiple equal-volume shells where larger sizes have more shells to accurately capture diffusion gradients.

representation of chips are converted from three-dimensional solids into equivalent volume spheres to simplify the spatial complexity of diffusion calculations. Resulting radial dimension is in turn discretized through concentric multiple shells, as depicted in Figure 2. Depending on the overall size of each thickness classification there can be an appropriate number of discrete shells to maintain spatial accuracy. Shells are chosen as equal-volume segments resulting in progressively thinner shells from the core to the outside surface.

(4) Solid chips, entrapped liquor in the porous matrix, and free liquor between chips are the three distinct phases in transport and reaction calculations. Liquor–solid reactions occur between solid shell segments and the entrapped liquor contained within. Diffusion between entrapped liquor segments of internal shells and the exchange between the outer shell and the free liquor determine liquor density (composition) for reactions.

(5) Solid compaction is a computed dynamic state for each plug that depends on chip conversion and pertinent hydrodynamic properties of the digester.

Solid Plugs and the Numerical Method

Perhaps the most distinguishing feature of the new model is the departure from the traditional multiple CSTR approximation of the tubular reactor behavior. For steady-state calculations there are obvious advantages of the consecutive CSTR compartmentalization of a plug flow reactor volume arising from the simple modeling requirements of the associated stationary spatial coordinates. However transient behavior is compromised with CSTR formulation, resulting in an overall artificial dispersion effect caused by the sequential filtering of any dynamic change through its progress as each CSTR acts like a first-order filter. In the new model presented here, a moving coordinate system convention is used to represent the transport of chips as multiple distinct plugs, as shown in Figure 3, where each plug has a time-dependent location coordinate. Input plug volumes are allowed to be flexible to accommodate variable feed rates while the makeup of each individual plug is preserved during its residence time in the digester, that is, there is no solids mixing between adjacent plugs. With this approach, each plug of chips travels through the digester system as a distinct entity undergoing transport and reaction dynamics much like a batch reactor of solids passing through changing liquid reactant environments. Plugs undergo both time- and space-dependent dynamics as the operating conditions dictate. Effective plug volumes, solid compactions, and instantaneous velocities constantly change in response to input–output rates,

local digester diameter, conversion of chips, and relative hydrodynamic forces. Entrapped liquor inside the chips travels with plugs while undergoing reaction- and transport-related changes, but the free liquor flow direction and speed, to which a plug is exposed, are dictated by the external flow rates and internal volumetric conservation constraints. Thus, a collection of involved yet manageable geometric details are introduced with the moving coordinate modeling approach to avoid the dynamic drawbacks of the otherwise simpler CSTR formulation.

The numerical method used to solve the model equations is relatively straightforward, where spatial and temporal dynamics are handled consecutively within incremental discrete times. A typical discrete time is 2 min, which provides sufficient accuracy over 4 to 6 h of digester residence time. Spatial dynamics of plug movements and compactions are solved as a constrained algebraic problem followed by the time-dependent transport and reaction calculations during the full incremental time period. Sequential incremental solution of system dynamics through a combination of instantaneous spatial movements followed by temporal variations is sometimes referred to as the *cinematic approach*.

Basic steps of the numerical algorithm for the new model can be briefly stated as:

(1) Initially fill digester and IV with solid plugs and liquor using a nominal plug size to render the desired numerical accuracy with reasonable computation times. Typically about 1200 plugs are used to fill both vessels.

(2) For the duration of discrete time period Δt and for each plug solve the corresponding transport and reaction related

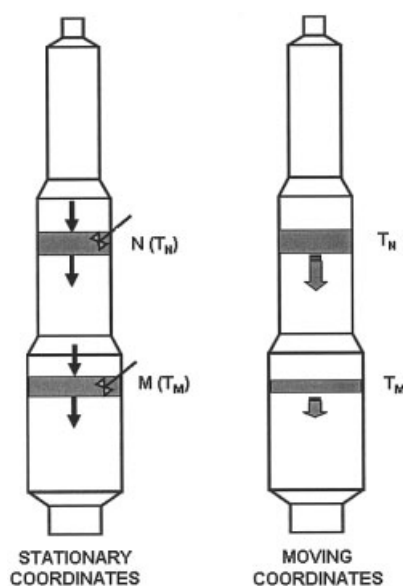


Figure 3. Moving coordinate system approach to capture accurate plug flow dynamics of chips compared to the more traditional sequential CSTR approach.

With solids flow passing through fixed-location CSTRs chip residence time distributions propagate with a widening dispersion around mean ages, such as T_N and T_M . On the other hand, moving discrete (volumetric) solid plugs maintain exact space time as the age of all chips contained in a plug.

ordinary differential equations to update chemical densities for solid, entrapped liquor, and free liquor phases.

(3) Introduce new solid plugs (chips) into the system to the IV and remove converted plugs (pulp) from the system at digester bottoms to match present flow conditions and other chip-level-control-related flow adjustments. Move solid plugs to maintain volume continuity. Compute solid compactions using plug hydrodynamic conditions and chip conversion, and rearrange effective plug volumes and locations. Compute free liquor movement in response to overall external liquor flow-rate decisions and the void space constraints imposed by plug movement.

(4) Increment time and go to step 2.

Model Equations

Governing material and energy balance equations of the new-generation model are similar to those reported by Wisniewski.⁵ Details will be kept to a minimum here because of space limitations. It is worth noting that, to track chip size and diffusion rate limitations, interparticle solid and liquor density gradients are calculated in a manner similar to that proposed by Gustafson,² compared to the lumped-parameter approach of Wisniewski. Furthermore, dynamic chip compaction calculations are done with similar assumptions and correlations as in Michelsen,⁶ which were originally proposed by Harkonen.⁸

Reaction rates for solid densities are specified as

$$R_{Si} = -\theta_i [k_{Ai}\rho_{L1} + k_{Bi}\rho_{L1}^{1/2}\rho_{L2}^{1/2}](\rho_{Si} - \rho_{Si}^\infty) \quad i = 1, \dots, 5 \quad (1)$$

with reaction rate constants defined as

$$k_{Ai} = k_{Aoi}\exp(-E_{Ai}/RT) \quad \text{and} \quad k_{Bi} = k_{Boi}\exp(-E_{Bi}/RT) \quad (2)$$

Liquor component rates are related through stoichiometric relationships as

$$R_{L1} = (\beta_{EAL}R_{LG} + \beta_{EAC}R_C)\left(\frac{1-\eta}{\eta}\right) \quad (3)$$

$$R_{L2} = (\beta_{HSL}R_{LG})\left(\frac{1-\eta}{\eta}\right) \quad (4)$$

$$R_{L3} = (-R_S)\left(\frac{1-\eta}{\eta}\right) \quad (5)$$

$$R_{L4} = (-R_{LG})\left(\frac{1-\eta}{\eta}\right) \quad (6)$$

where $R_{LG} = R_{S1} + R_{S2}$, $R_C = R_{S3} + R_{S4} + R_{S5}$, and $R_S = R_{LG} + R_C$.

Entrapped liquor density diffusion coefficient is

$$D = \theta_2 8 \times 10^{-8} T^{1/2} \exp(-2450/T) \quad (7)$$

Chip compaction under pressure is given by the Harkonen⁸ correlations, where solid conversion is related to a conventional relation for flow pressure drop in two-phase media:

$$\eta = 0.644 - [0.831 - 0.139 \ln(\text{Kappa})](P/10)^{0.59}$$

$$-\frac{\Delta P}{L} = 4.6 \left(\frac{1-\eta}{\eta}\right)^2 \nu + 3900 \left(\frac{1-\eta}{\eta}\right) \nu^2 \quad (8)$$

Internal chip transport and reaction rates are computed by material balances around concentric spherical shells as shown in Figure 2. A typical set of model equations for shell “ m ” as numbered from inside to outside ($1, \dots, m, \dots, M$) are as follows:

Solid component balances for $i = 1, \dots, 5$ and $m = 1, \dots, M$ are

$$\frac{d\rho_{sim}}{dt} = R_{sim} \quad (9)$$

Entrapped liquor component balances for $j = 1, \dots, 4$ and $m = 2, \dots, M - 1$ (with appropriate modifications for $m = 1$ and M) are

$$\frac{d\rho_{Ljm}^e}{dt} = R_{Ljm}^e + \alpha_{m,m}\rho_{Ljm+1}^e - (\alpha_{m,m} + \alpha_{m,m-1})\rho_{Ljm}^e + \alpha_{m,m-1}\rho_{Ljm-1}^e \quad (10)$$

where

$$\alpha_{m,m} = \frac{a_m D}{v_m(r_{m+1} - r_m)} \quad (11)$$

and

$$\alpha_{m,m-1} = \frac{a_{m-1} D}{v_m(r_m - r_{m-1})} \quad (12)$$

and where superscript e designates the entrapped liquor properties (as opposed to free liquor); a_m is the external (toward outside) surface area of a shell; v_m is the volume of a shell; and r_m is the half mass (volume) radius of a shell representing bulk density point.

Free liquor material balances are determined from the cumulative diffusion rates of the outer shells from each size cut.

Nomenclature and nominal parametric values are listed in the notation section. The nominal values provided here are the previously established³ basic references and may need to be reassessed and appropriately adjusted for each practical application.

Mill Case Studies

Model customization

The model was customized for a specific digester essentially by matching the physical dimensions of the two vessels, including metal thickness for thermal transient calculations, and

by providing corresponding input and output flow structures so that process operating decisions of the software code would emulate real operator decisions. Physical properties of chip species were basically known from literature. However, the specific size (thickness) distribution data were obtained from the mill's weekly averaged chip-feed quality reports. Tuning of the model was accomplished by matching simulated results to historic operating data where selected quasi-steady-state data representing multiple production rates over a 6-month period were used to adjust only one model parameter, the reaction rate effectiveness factor θ_1 (see Eq. 1 and Notation and Symbols section). Additional model customizations included improved graphical user interface details for model inputs and outputs so that the mill engineers could intuitively interact with the software.

Model validation

Upon constructing a customized model of the digester, a series of validation tests were performed. Every morning, the current mill operating conditions were entered into the model and digester performance conditions (such as blowline Kappa number, residual EA) were compared with the model predictions to determine whether the model was behaving in a manner analogous to the mill conditions. After 3 months of validation studies, it was determined that the model was accurately predicting the performance of the digester under fairly standard mill operating conditions.

Process improvement

Once the model was validated by accurately predicting several months' worth of measurable operating conditions, the predicted Kappa number, free liquor residual EA, chip differential pressure, temperature, and column compaction profiles were used to help visualize the operating conditions over the entire length of the digester. An examination of the calculated profiles indicated that the mill was operating under less than ideal conditions. A significant discontinuity existed in the predicted residual alkali profile. The residual alkali was predicted to be critically low near the lower extraction zone and a delignification dead zone was hypothesized in the MCC portion of the digester. The chip-compaction profile suggested that the digester was operating near a hanging condition that would impede chip column movement. Additionally, a reasonably large Kappa number variability was predicted to exist as a result of improperly balanced cooking (reaction) conditions.

The model inputs were varied to obtain operating conditions that alleviated these predicted deficiencies in the calculated process profiles while maintaining the desired output Kappa number. The EMCC digester maintains the ability to input white liquor at four distinct points: the IV, the BC Sluice, the MCC section, and at the Wash zone. The original operating conditions used 60% of the white liquor in the IV, 15% in the BC Sluice, 20% in the MCC section, and 5% in the Wash zone. To improve the delignification (Kappa number) profile, the free liquor residual EA profile, and the hydraulic profile throughout the digester column, it was decided that significant amounts of white liquor needed to be shifted from the front end of the digester toward the middle of the digester column. The liquor that was used in the BC Sluice was split between the IV and the

MCC and Wash zone. The optimized model shifted a portion of the white liquor from the BC Sluice to the IV to increase the effective liquor penetration into the chip. The remaining portion was split between the MCC and the Wash zone. After these changes were made to the model, the improved liquor splits used were 65, 0, 28, and 7% in the IV, BC Sluice, MCC, and Wash zone, respectively.

Operating the new liquor splits with the same amount of total applied white liquor was predicted to result in desired changes in the cooking profile of the digester. The model predicted that more of the white liquor would be consumed in a much gentler, more uniform cooking profile. At the end of the cook zone, the original cooking conditions were predicted to produce a pulp with a 55 Kappa number and final Kappa number of 20.0. The modified liquor split condition was predicted to produce a Kappa number of 63 at the end of the cook zone and a final Kappa number of 17.2. The total extract-free liquor residual EA was predicted to decrease from 5.2 to 4.8 g/L.

Once reasonable cooking, free liquor residual EA, and differential pressure profiles were established, the temperature profile was manipulated to return the predicted output (blowline) Kappa number to the mill target of 21. Several degrees were eliminated from the Cook, MCC, and Wash zone temperatures to obtain the desired predicted Kappa number with the new liquor splits.

The optimized liquor splits used in the model were implemented in the mill. Almost immediately, the blowline Kappa number and the residual EA in the extraction dropped. Instead of using the temperature profile indicated by the model, the mill opted to use a different profile where significant temperature cuts performed in the bottom circulation zone of the digester only. These new operating conditions were used for several months and resulted in smoother, more uniform operation of the digester. By altering the liquor splits and temperature profiles of the digester the mill was able to reduce the Kappa number standard deviation in the blow line pulp by at least 5 Kappa points.

Diagnostics and troubleshooting

Shortly after a major mill-wide outage, the digester started producing higher than normal Kappa number pulps with a very large standard deviation. Instead of producing 19–20 Kappa number pulp, the digester was producing pulps in the 30 Kappa number range with intermittent Kappa swings between 15 and 45. According to the available instrumentation, the operating conditions had not changed. Initial checks of the instrumentation and digester controls indicated that everything was operating well within design parameters. Because the output results were not normal and relatively unstable, it was decided that an intermittent problem had to exist in the instrumentation.

Various potential conditions were examined with the model in an attempt to simulate the higher than normal Kappa number typically experienced in the mill. One controllable input parameter was significantly altered at a time in an attempt to simulate the current mill operating conditions. The model results suggested that a problem existed with the wash zone operating temperature. To obtain the higher than normal Kappa numbers in the model predictions, the wash zone temperature in the model had to be lowered from the standard operating condition of 338 to 250°F with all of the other controllable

input parameters being held constant, thus indicating high probability of the root cause for the problem. Close examination of the temperature probes in the digester revealed the wash zone temperature probe was in fact providing intermittently bad signals to the temperature-control software. Once this probe was replaced, the digester returned to its normal and expected behavior.

Conclusions

A new-generation continuous digester model is developed to provide high-fidelity simulation capabilities specifically suitable for species and rate transition dynamics. Undesirable filtering effects of CSTR approximation are avoided by using multiple moving solid plugs with a customized numerical algorithm that deals with spatial and temporal dynamics in a sequential manner. Dynamic compaction and chip size distribution effects are easily incorporated in the model. On a Pentium-4 3.2-GHz PC the model operates at a speed about 300 times faster than real process time. The model predicts informative operating conditions such as internal chip conversion, residual alkali, and dissolved solids profiles, which cannot be measured in a production environment but are very useful for revealing details for process improvement decisions. The model has been successfully used to develop improved mill operating conditions and to predict the location of instrumentation problems. To date, excellent correlation has existed between model predictions and mill results.

Notation and Symbols

- β_{EAC} = stoichiometric coefficient for mass of effective alkali (EA) consumed/mass of reacting carbohydrate: softwood value = 0.395; hardwood value = 0.49
- β_{EAL} = stoichiometric coefficient for mass of effective alkali consumed/mass of reacting lignin: softwood value = 0.166; hardwood value = 0.21
- β_{HSL} = stoichiometric coefficient for mass of hydrosulfide (SH^-) consumed/mass of reacting lignin: softwood value = 0.039; hardwood value = 0.05
- D = diffusivity, m^2/min
- E_{Ai} = activation energies, $i = 1, \dots, 5$ (kJ/gmol): softwood values [29.3 115 34.7 25.1 73.3]; hardwood values [29.3 115 34.7 25.1 73.3]
- E_{Bi} = activation energies, $i = 1, \dots, 5$ (kJ/gmol): softwood values [31.4 37.7 41.9 37.7 167]; hardwood values [31.4 37.7 41.9 37.7 167]
- EA = effective alkali, concentration of NaOH and Na_2S expressed as equivalent Na_2O , g/L or kg/m^3
- η = volume fraction of liquor, compaction

- Kappa # = Kappa number = $654 \times \text{lignin mass}/\text{total solid mass}$
- k_{Aoi} = preexponential factors ($\text{m}^3 \text{ liq}/\text{min}^{-1} \text{ kg}_{\text{EA}}^{-1}$): softwood values [0.2809 6.035 $\times 10^{10}$ 6.4509 1.5607 10197]; hardwood values [0.3954 1.457 $\times 10^{11}$ 28.09 7.075 5826.7]
- k_{Boi} = preexponential factors [$\text{m}^3 \text{ liq}/\text{min} (\text{kg}_{\text{EA}} \text{ kg}_{\text{EA}})^{-1/2}$]: softwood values [9.26 0.489 28.09 10.41 5.722 $\times 10^{16}$]; hardwood values [12.49 1.873 124.9 47.86 3.225 $\times 10^{16}$]
- θ_1 = reaction rate effectiveness factor
- θ_2 = diffusion rate effectiveness factor
- ρ_{Lj} = liquor component densities, $j = 1, \dots, 4$ (kg/m^3 of liquor); indices are respectively: effective alkali (EA), hydrosulfide (SH^-), dissolved solids, and dissolved lignin
- ρ_{Si} = solid component densities, $i = 1, \dots, 5$ (kg/m^3 of solid); indices are respectively: high reactivity lignin, low reactivity lignin, carbohydrate, galactoglucomannan, and araboxylan
- ρ_{Soi} = solid component densities in wood chips (kg/m^3 of solid); softwood values [72 280 755 33 360]; hardwood values [150 225 675 75 375]
- ρ_{Si}^∞ = unreactive portion of solid component densities in wood chips (kg/m^3 of solid): softwood values [0 0 435 18 0]; hardwood values [0 0 535 18 0]
- P = chip (column) pressure, kPa
- $\Delta P/L$ = pressure drop, kPa/m
- R = gas constant ($\text{kJ gmol}^{-1} \text{ K}^{-1}$) = 0.0083144
- R_{Lj} = reaction rate of liquor component j , (kg/min)/(m^3 of liquor)
- R_{Si} = reaction rate of solid component i , (kg/min)/(m^3 of solid)
- T = temperature, K
- v = relative fluid velocity, m/s

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