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Thermal-Hydraulic Digester Model Using A Higher Order Numerical Method

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Motivation

- Chip level control
 - Digester endpoint Kappa # (Amirthalingam & Lee, 2000)
- Grade transition control
 - Hardwood/softwood swings
- Process monitoring and fault diagnosis

Development of a fundamental model based on mass, heat and momentum conservation



Literature Overview: Fundamental Continuous Digester Models - Purdue Model

- 1974 — Smith and Williams
Series of CSTRs, 3 phase system, kinetic parameters
- 1982 — Christensen *et al.*
*Optimal kinetic parameters, specie rate multiplier,
mass transfer data*
- 1986 — Maras *et al.*
Thermal balance for wood and liquor
- 1996 — Kayihan *et al.*
2-vessel model
- 1997 — Wisniewski *et al.*
Improved defns. of mass conc. and volume fractions
- ↓



Literature Overview: Fundamental Continuous Digester Models

1987 — Härkönen
Chip compaction, velocity - hydraulics

1995 — Michelsen
Hydraulics + simplified Purdue kinetics

↓

- Gustafson and co-workers > 1983
Kinetics, detailed diffusion, chip size distribution



Perspective

Past models

Purdue

*Smith, Christensen,
Wisniewski et al.
(1974, 1982, 1997)*

Michelsen (1995)

Mass/Energy

Mass/Energy/Momentum

High fidelity kinetics

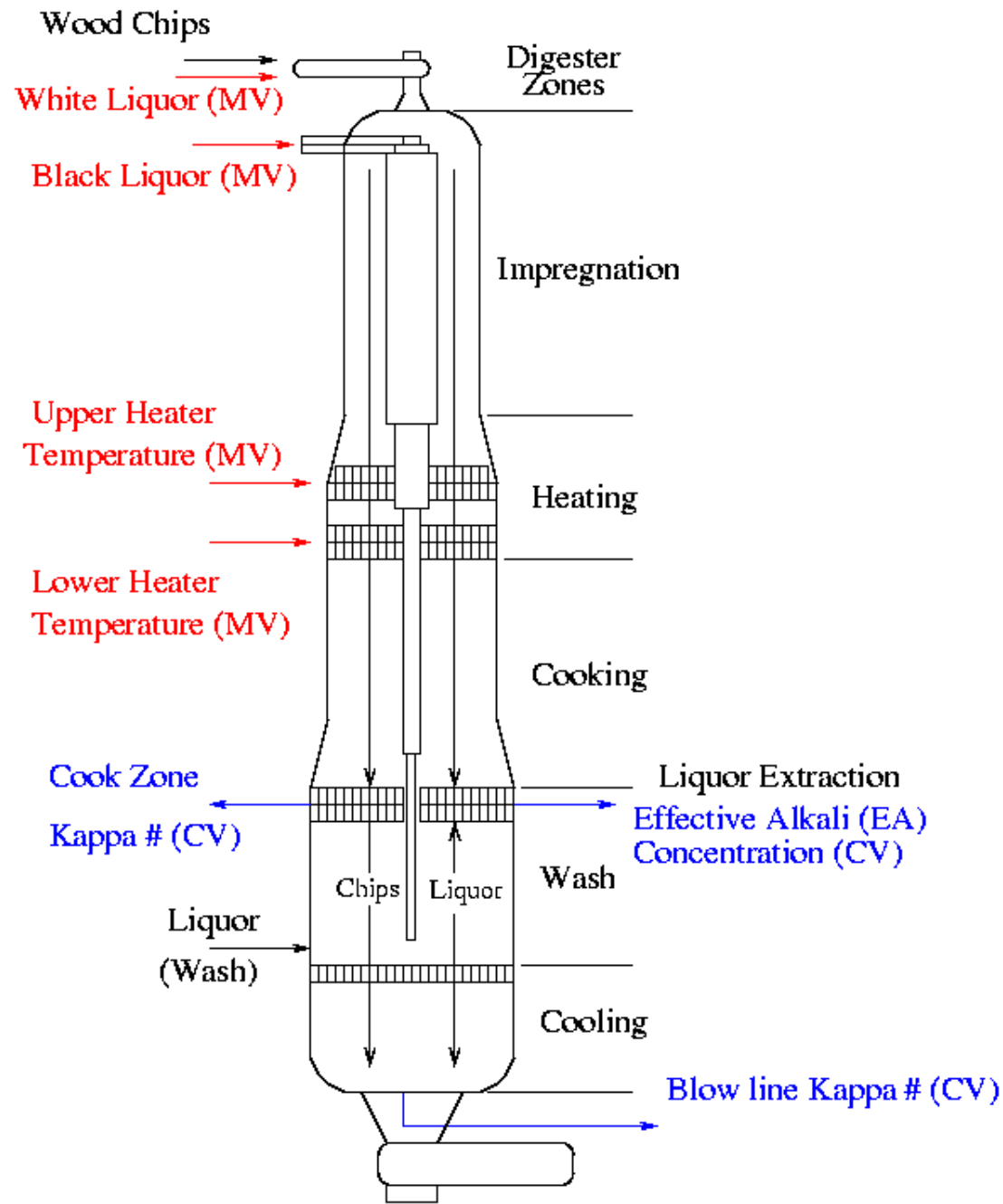
Level/compaction profile

No level, fixed compaction

Valid for (50-150) K# range

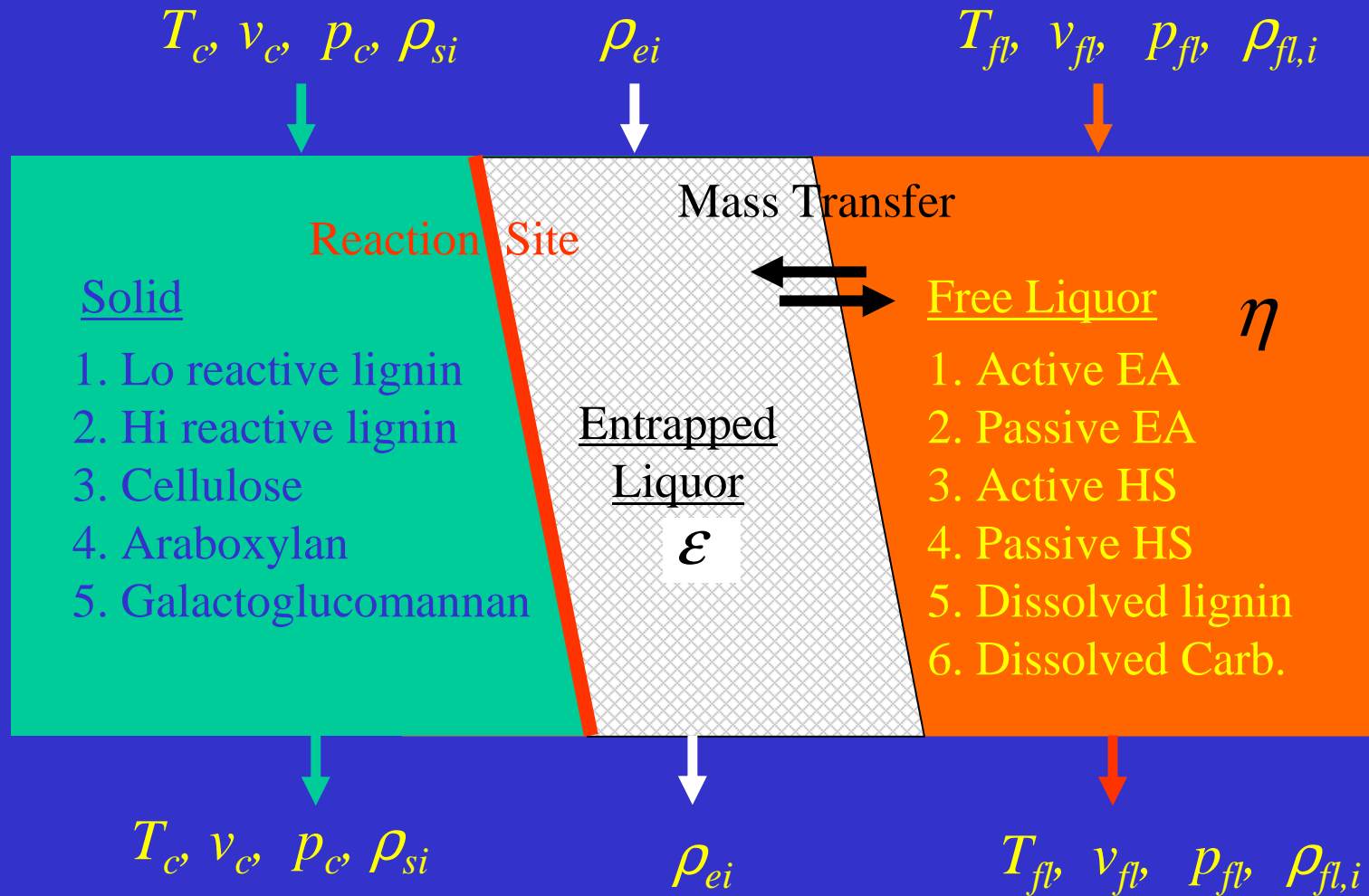
- Thermal-hydraulic Purdue Model
- Higher Order Numerical Method

Current Work





Model





Summary of Assumptions

- Radial property gradients neglected (*P, M*)
- Solid/entrapped phase in thermal and dynamic equilibria (*M*)
- Stratified, incompressible flow (*P, M*)
- Liquor-wall resistance neglected (correlation/experimental data) (*M*)
- Acceleration of liquor negligible (simplified) (*M*)
- Constant cross-sectional area (*M*)
- Pulping chemistry based on McKibbins (1960)
- Hydraulic constitutive laws based on Härkönen (1987)

P - Purdue
M - Michelsen



Mass Continuity

Solid Phase

$$\frac{\partial \rho_{si}}{\partial t} = -v_c \frac{\partial \rho_{si}}{\partial z} + \hat{R}_{si}$$

Bulk flow Reaction

Entrapped Liquor Phase

$$\frac{\partial \rho_{ei}}{\partial t} = -\frac{\rho_{ei}}{\varepsilon} \frac{\partial \varepsilon}{\partial t} + \frac{v_c}{\varepsilon} \frac{\partial (\varepsilon \rho_{ei})}{\partial z} + D(\rho_{fi} - \rho_{ei}) + \hat{R}_{ei}$$

Bulk flow Diffusion Reaction

Free Liquor Phase

$$\frac{\partial \rho_{fi}}{\partial t} = -v_c \frac{\partial \rho_{fi}}{\partial z} - D\varepsilon \frac{(1-\eta)}{\eta} (\rho_{fi} - \rho_{ei}) \pm \rho_{fi,ext} \frac{\dot{V}_{ext}}{\delta V_f}$$

Bulk flow

Diffusion

External flows

recirculation/extracts



Volume Continuity

Chip Phase Volume Continuity

$$\frac{\partial \eta}{\partial t} = \frac{\partial}{\partial z} [(1 - \eta)v_c]$$

Overall Digester Volume Continuity

$$\nabla_z (\dot{V}_c + \dot{V}_f) = 0$$

Space not occupied by chips must be filled with liquor



Momentum Conservation

Chip Phase

Bulk
momentum

Chip
pressure

Liquor
pressure

Chip/liquor flow
resistance

$$\rho_c(1-\eta)\frac{\partial v_c}{\partial t} = -v_c(1-\eta)\rho_c\frac{\partial v_c}{\partial z} + \rho_c(1-\eta)g - \frac{\partial p_c}{\partial z} - (1-\eta)\frac{\partial p_f}{\partial z} - F_\Lambda - F_\mu$$

Gravity

Chip/wall friction

Liquor Phase

$$\frac{\partial p_f}{\partial z} = -v_f\frac{\partial}{\partial z}[\rho_f v_f] - \eta v_f\frac{\partial \rho_f}{\partial t} + \rho_f g + \frac{F_\Lambda}{\eta}$$

Gravity

Chip/liquor flow
resistance



Energy Conservation

Chip Phase

$$(C_{Ps}M_s + C_{Pe}M_e\epsilon) \frac{\partial T_c}{\partial t} = -T_c \left(C_{Ps} \frac{\partial M_s}{\partial t} + C_{Pe} \frac{\partial (M_e\epsilon)}{\partial t} \right) - v_c \frac{\partial}{\partial z} [(C_{Ps}M_s + C_{Pe}M_e\epsilon)T_c] + \Delta H_R \sum_{i=1}^5 \hat{R}_{si} + U(T_f - T_c) + D\epsilon D_E$$

Diffusive energy

Bulk

Heat of reaction

Interphase heat transfer

Liquor Phase

$$C_{Pf}M_f \frac{\partial T_f}{\partial t} = -T_f \frac{\partial}{\partial t} (C_{Pf}M_f) \mp v_f \frac{\partial}{\partial z} (C_{Pf}M_f T_f) - U \frac{(1-\eta)}{\eta} (T_f - T_c) + \frac{D\epsilon D_E}{\eta} \pm \frac{\dot{V}_{ext} M_{ext} T_{ext}}{\delta V_f}$$

Diffusive energy

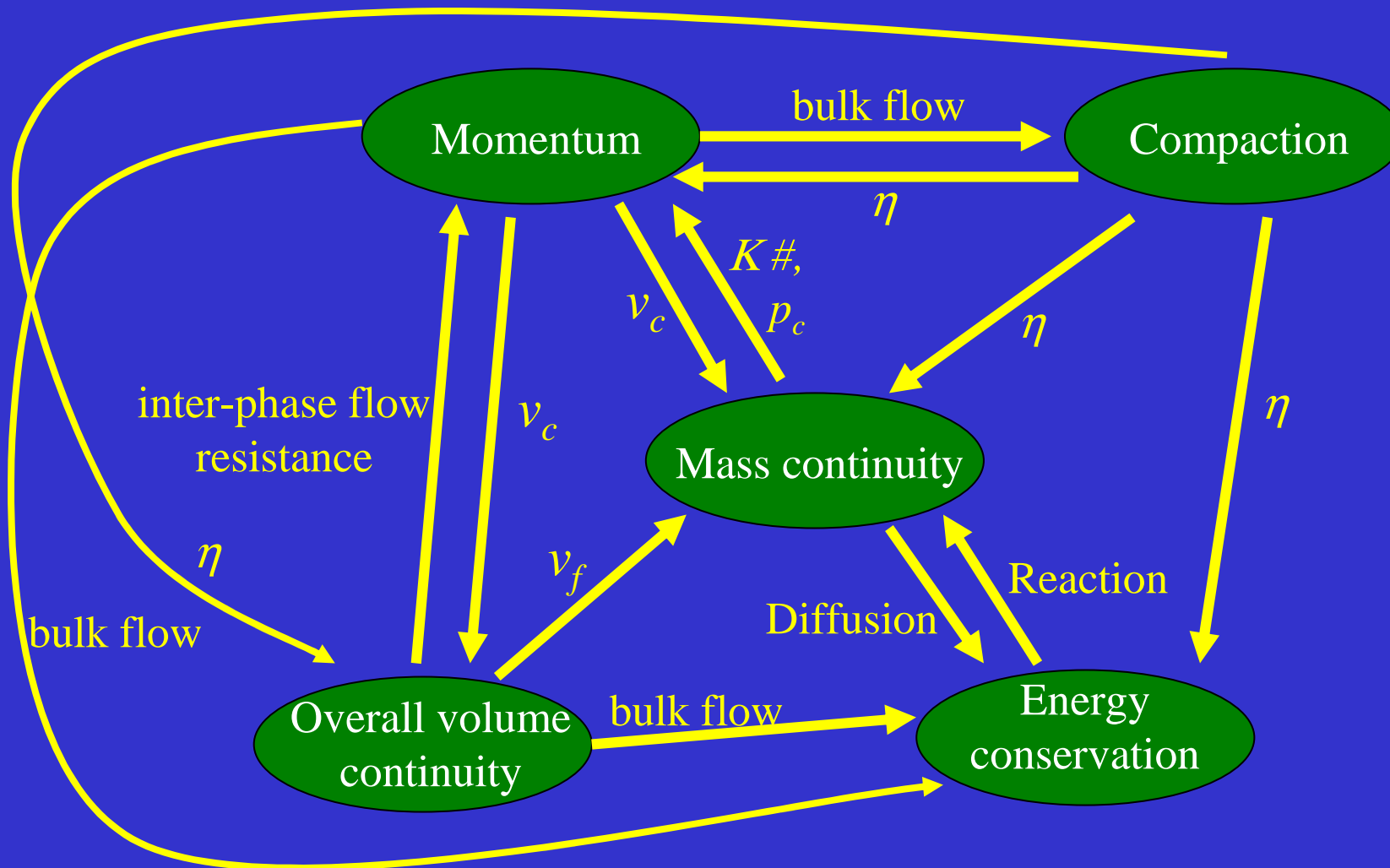
External flow

9





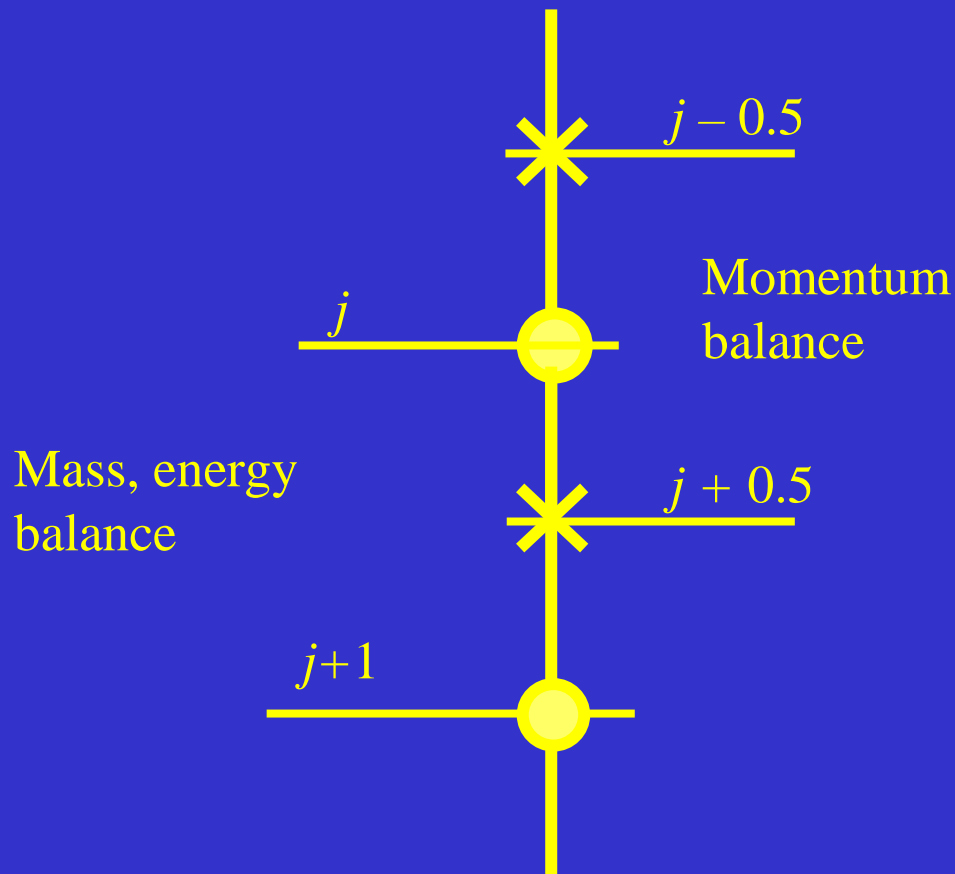
Phenomenological Interactions





Computational Issues

Staggered Grid (*Patankar, 1980*)



- 96 control volumes (CVs)
- Height: 0.29 m /CV
- 2213 states
- All variable properties vary linearly

Simulation Time

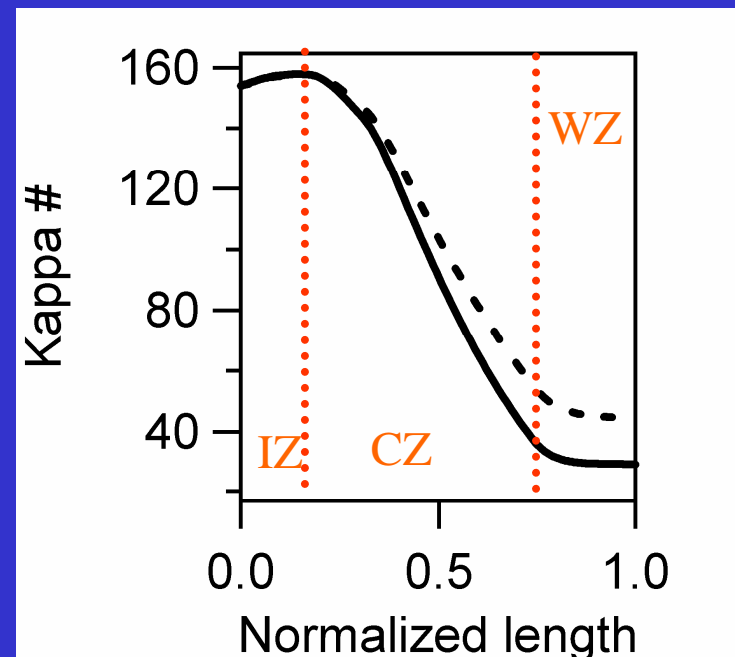
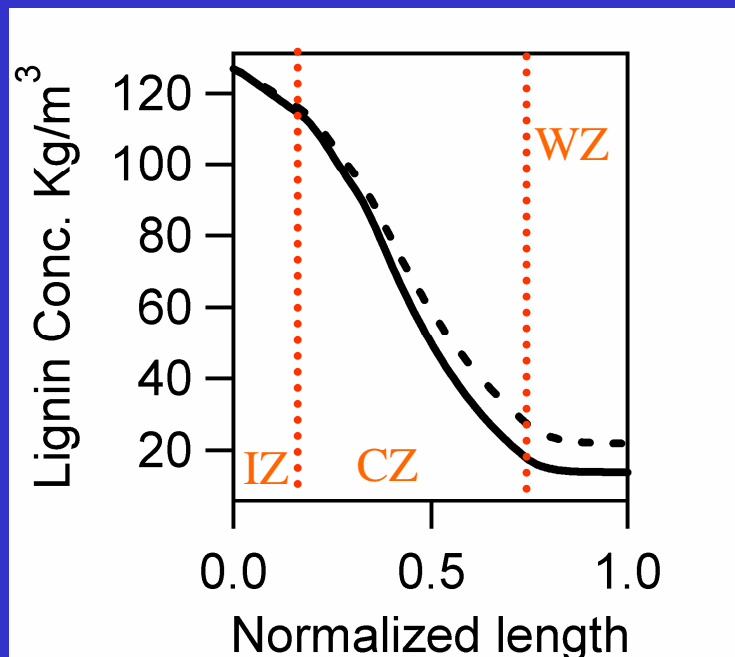
80 hr sim time - 25 min. real time

Sun Sparc Ultra 10 - 333Mhz



Production Rate Change

- Simultaneous chip feed and blow rate change
- Flow rate change of $\approx 11\%$ from nominal value
- Step change filtered using first order filter with 13 min. time constant



LPR

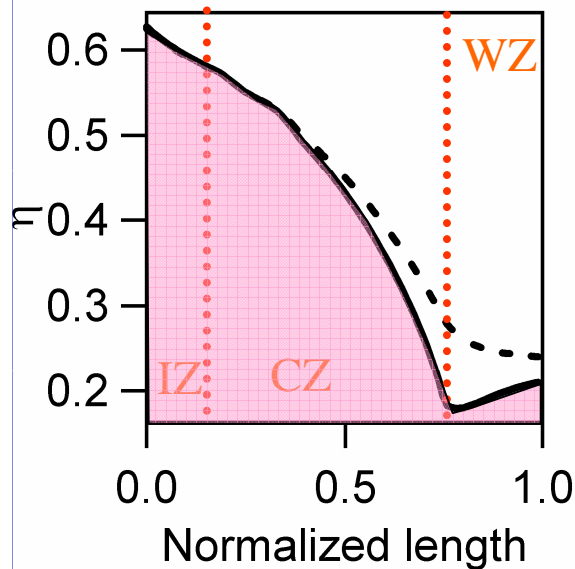
HPR



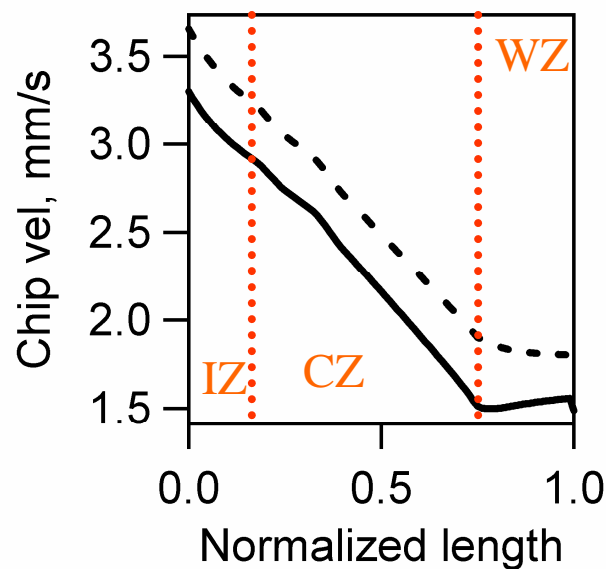
Steady-state Spatial Profiles

—— LPR
- - - HPR

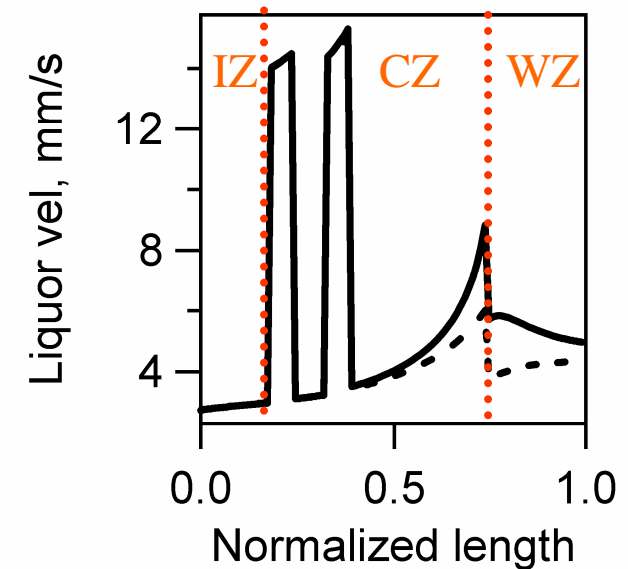
Compaction



Chip Velocity

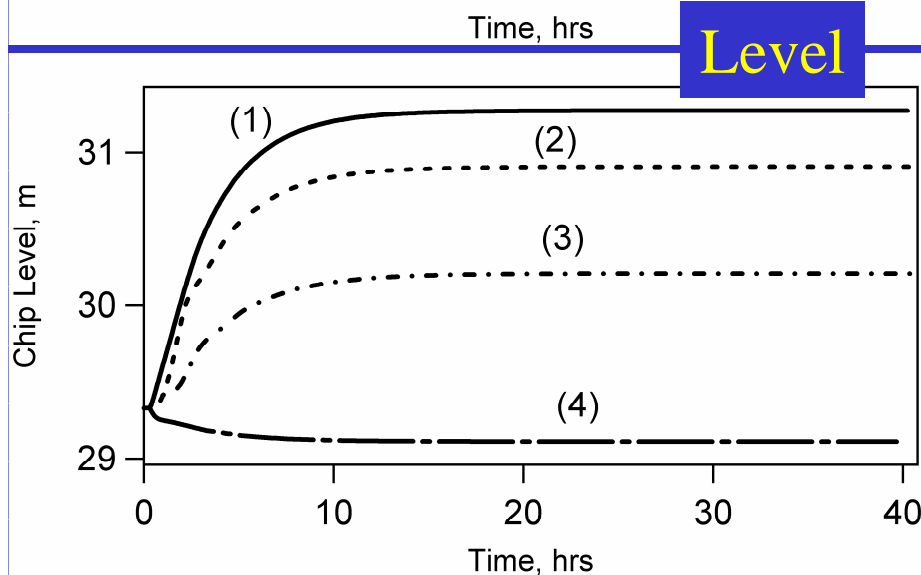
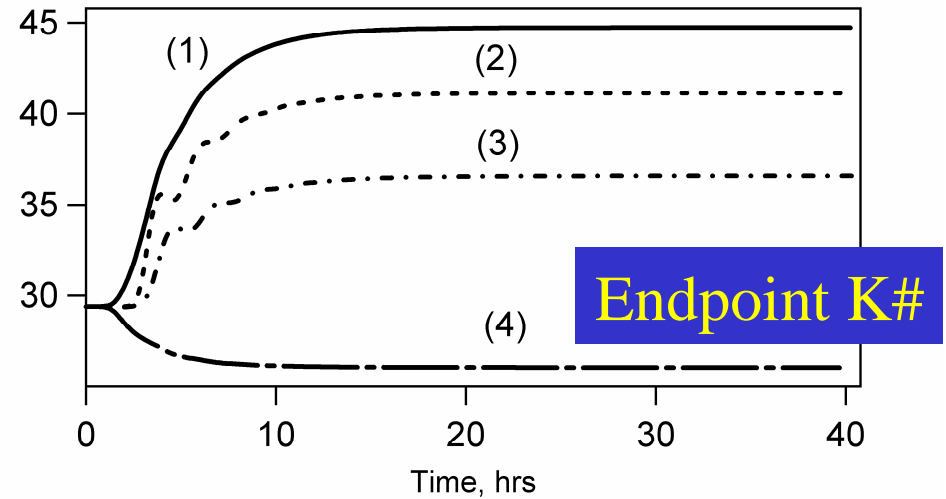
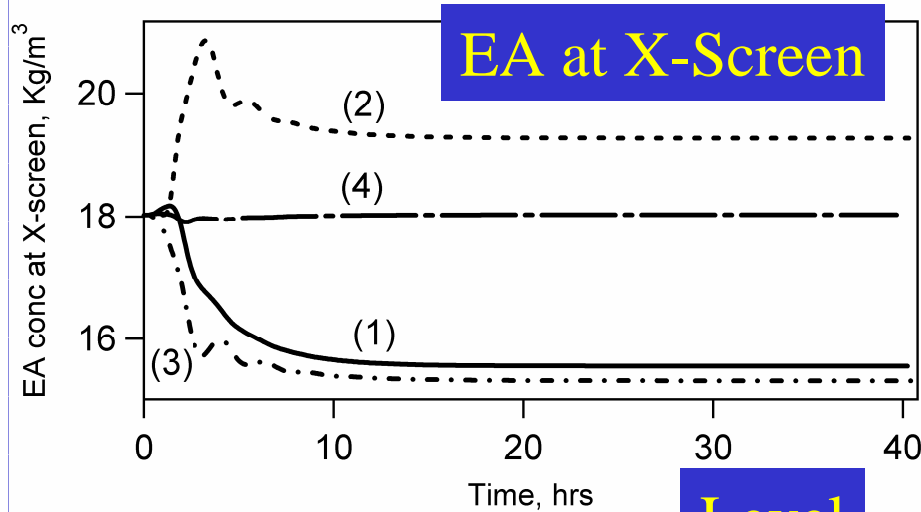


Liquor Velocity





Transient Response



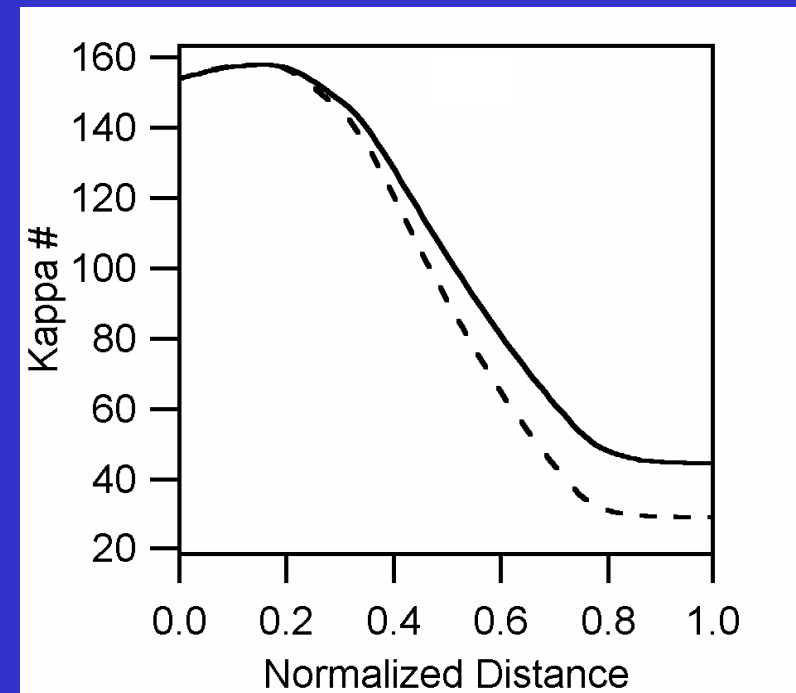
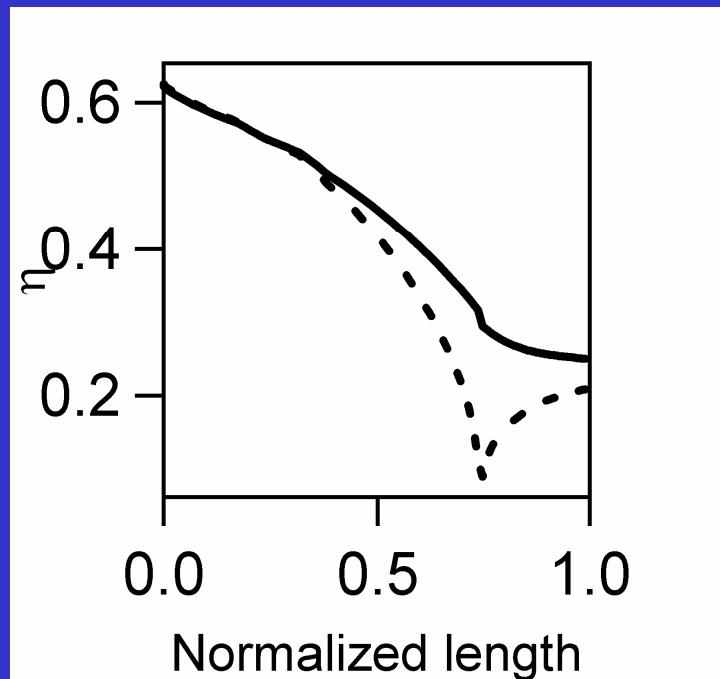
- (1) \uparrow in production rate
- (2) \downarrow in upper heater temperature
- (3) \downarrow in white liquor flow
- (4) \downarrow in dilute liquor flow



Near-Fault Scenario

- Step increase in white liquor flow

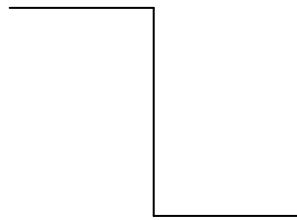
—— initial
- - - final



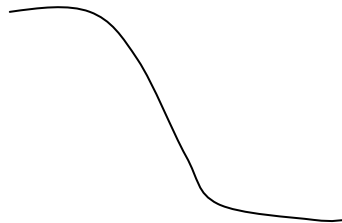


Higher Order Finite Difference

- Previous results based on first order finite differences (error $\sim O(h)$)
- Finite differences induces numerical diffusion in convective flows

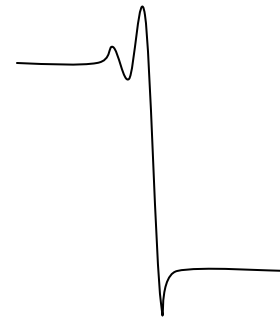


Exact Solution



Dissipation

(typical of odd order)



Dispersion

(typical of even order)

- *Approach*: First order at extremities and 4th order (error $\sim O(h^4)$) in between



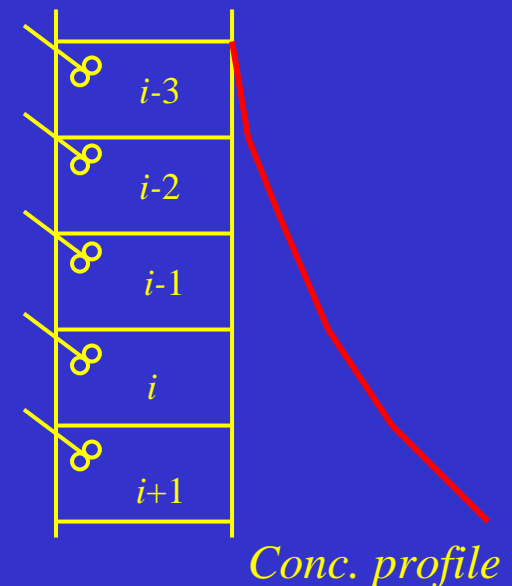
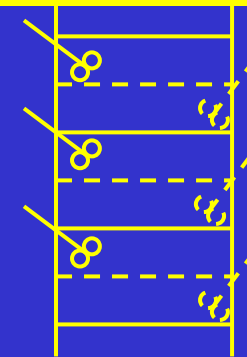
Enhanced Approximations For Plug Flow Using Finite Differences

- 1) Increase number of CSTRs
 - increases number of model states

- 2) Use higher order information for approximation

$$\frac{du_i}{dz} = \frac{-u_{i-3} + 6u_{i-2} - 18u_{i-1} + 10u_i + 3u_{i+1}}{12}$$

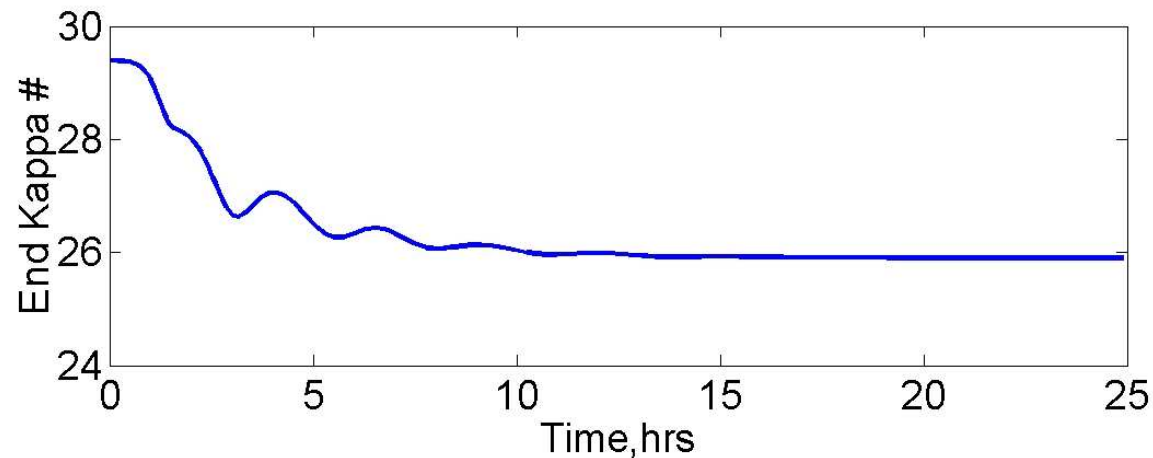
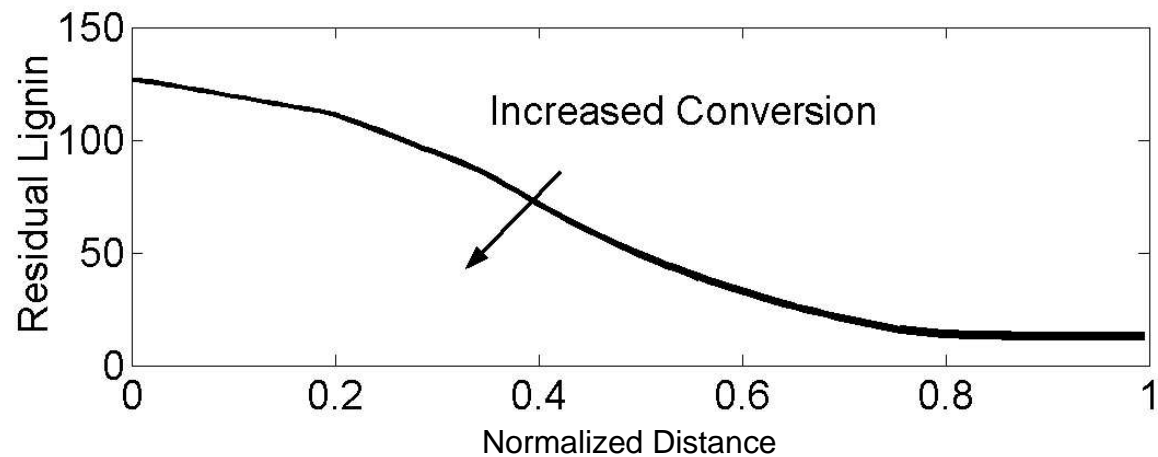
- *For the same volume, plug flow reactor shows higher conversion than CSTR*





Higher Order Numerical Method

- Better approximation of plug flow leads to lower Kappa #





Conclusions & Future Work

- A hydraulic extension of Purdue Model is presented
- Momentum transfer impacts $K \#$ and compaction profiles
- Simulation examples demonstrate coupling between momentum transfer and pulp quality profile
- A hybrid first/fourth order finite difference approximation shows increased conversion

- *Hardwood/softwood grade transition model extension*
- *Kappa profile control in a continuous pulp digester*



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