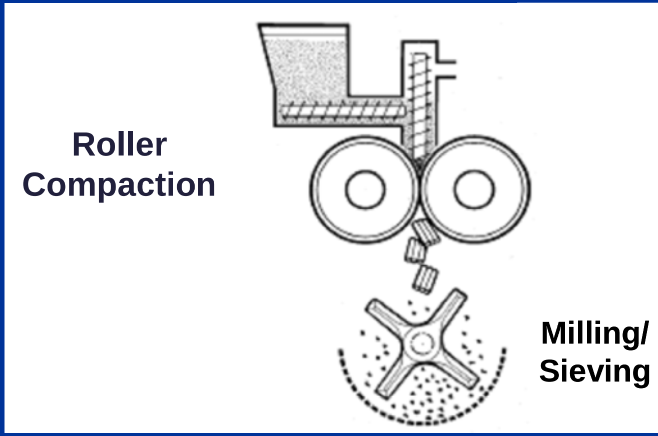
Dynamic Simulation of Roller Compaction

Shuo-Huan Hsu, Gintaras V. Reklaitis, Venkat Venkatasubramanian

Purdue University

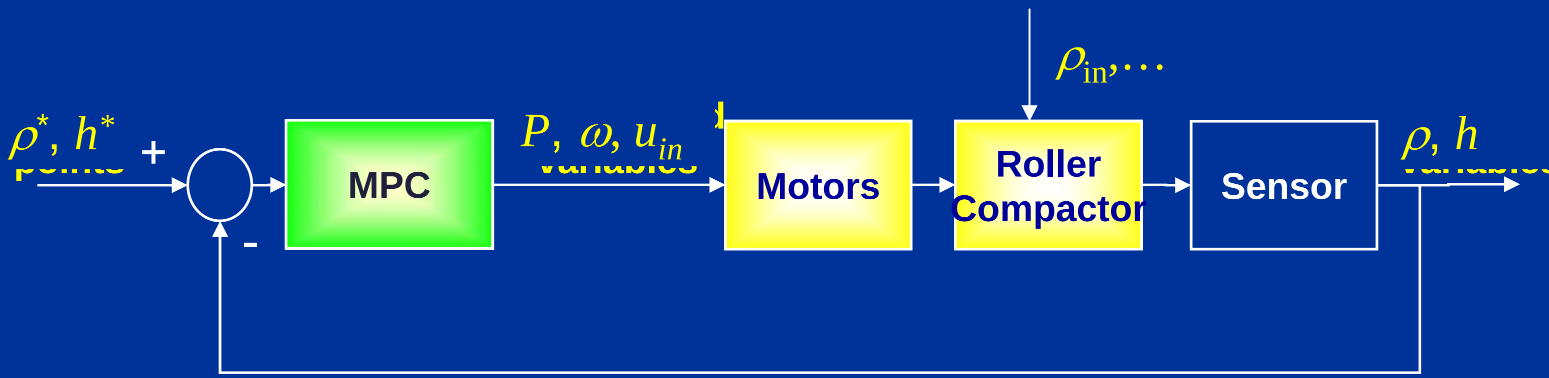
Dry Granulation

- Granulation → Increase/redistribute the particle size
  - Prevent segregation of the constituents of powder mix
  - Improve the flow properties and compaction characteristics
  - Dust problems are minimized
- Dry granulation
  - Attractive for moisture or heat sensitive pharmaceutical products
  - Roller compaction + mill
  - Compare with wet granulation
    - No solvent is used
    - Minimum energy consumption



- Optimal operation using process control techniques

Feedback Control



- Controller
  - Ensure the process runs safely and the product quality meets the requirement
- Controller design
  - Need to understand the process dynamics
    - How does the measurement change when the process variables vary?
    - Fast response
  - Mathematical model with **time dependency**

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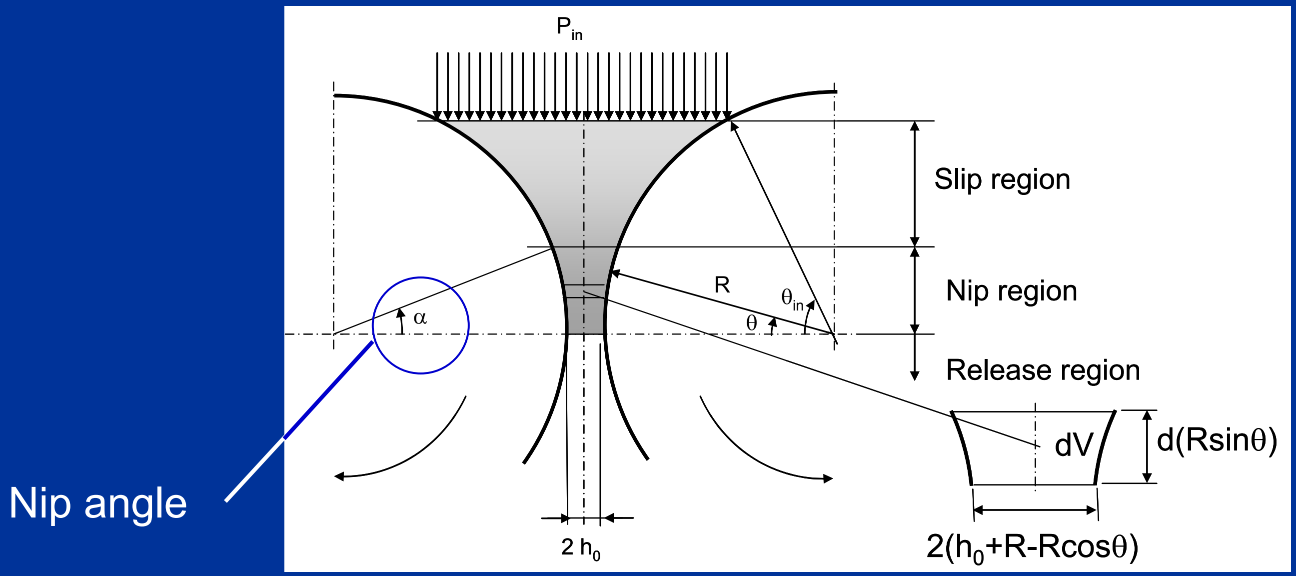
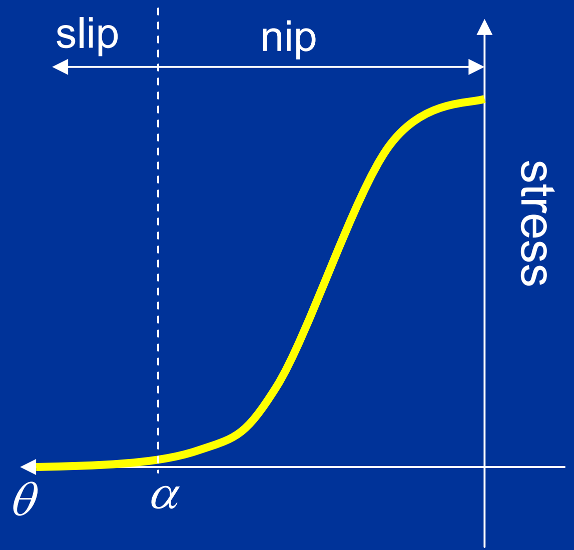
Johanson's Rolling Theory (1965)





- Predict the stress distribution of the particles
- Fixed gap size (h_0) → Steady state operation
- Different compression behaviors in different regions
- Material is
  - Isotropic, cohesive, compressible

Stress and Density Profile

- Slip region
  - Jenike and Shield effective yield function (1959)

$$\frac{d\sigma}{d\theta} = -\frac{4\sigma\left(\frac{\pi}{2}-\theta-\nu\right)\tan\delta}{\left(1+\frac{h_0}{R}-\cos\theta\right)\left[\cot(B-\mu)-\cot(B+\mu)\right]}$$

$$\mu = \frac{\pi}{4}-\frac{\delta}{2},\ \nu = \frac{1}{2}\left(\pi-\sin^{-1}\frac{\sin\phi}{\sin\delta}-\phi\right),\ B = \frac{1}{2}\left(\frac{\pi}{2}+\theta+\nu\right)$$

ϕ, δ: friction angles

- Nip region
  - Empirical model

$$\frac{\sigma(\theta)}{\sigma(\alpha)} = \left[\frac{\left(1+\frac{h_0}{R}-\cos\alpha\right)\cos\alpha}{\left(1+\frac{h_0}{R}-\cos\theta\right)\cos\theta}\right]^K, \quad \sigma = C_1\rho^K$$

C_1, K: parameters in the empirical model

- Nip angle, α

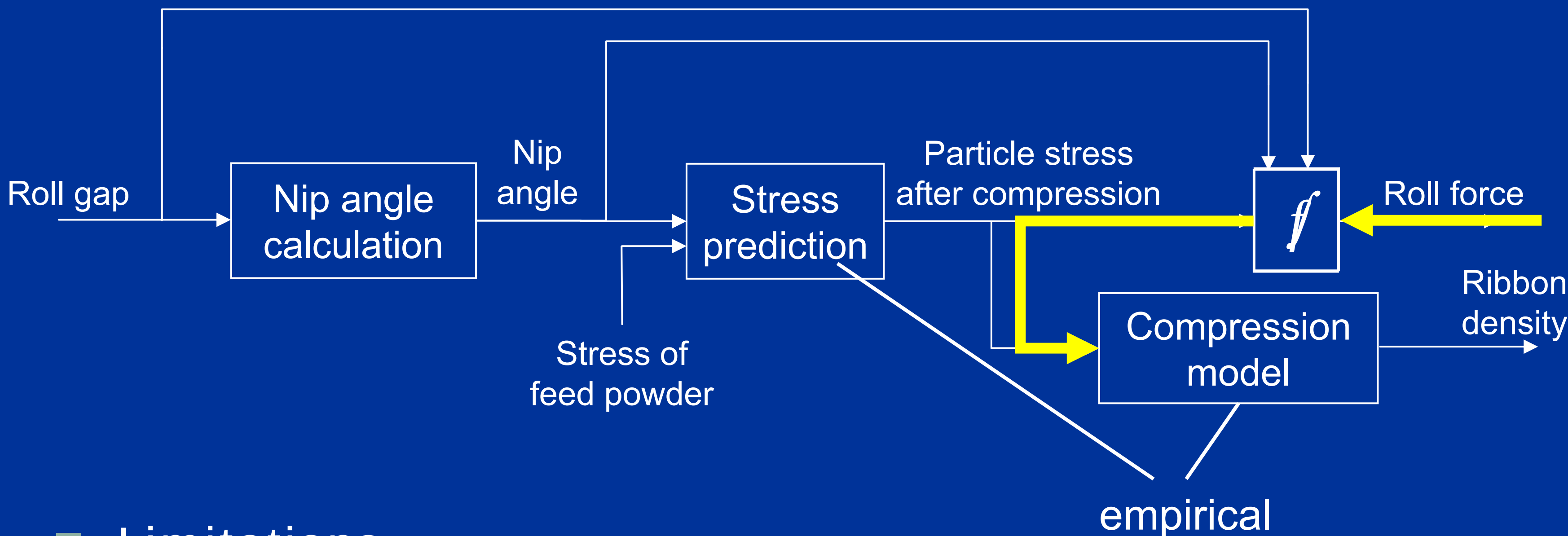
$$\left(\frac{d\sigma}{d\theta}\right)_{\text{slip}} = \left(\frac{d\sigma}{d\theta}\right)_{\text{nip}} @\,\theta=\alpha$$

- Roll Force, F (Force per ribbon width)

$$F = \frac{\sigma_{\text{exit}}R}{1+\sin\delta}\int_0^{\alpha}\left[\frac{h_0/R}{(1+h_0/R-\cos\theta)\cos\theta}\right]^K\cos\theta\, d\theta$$

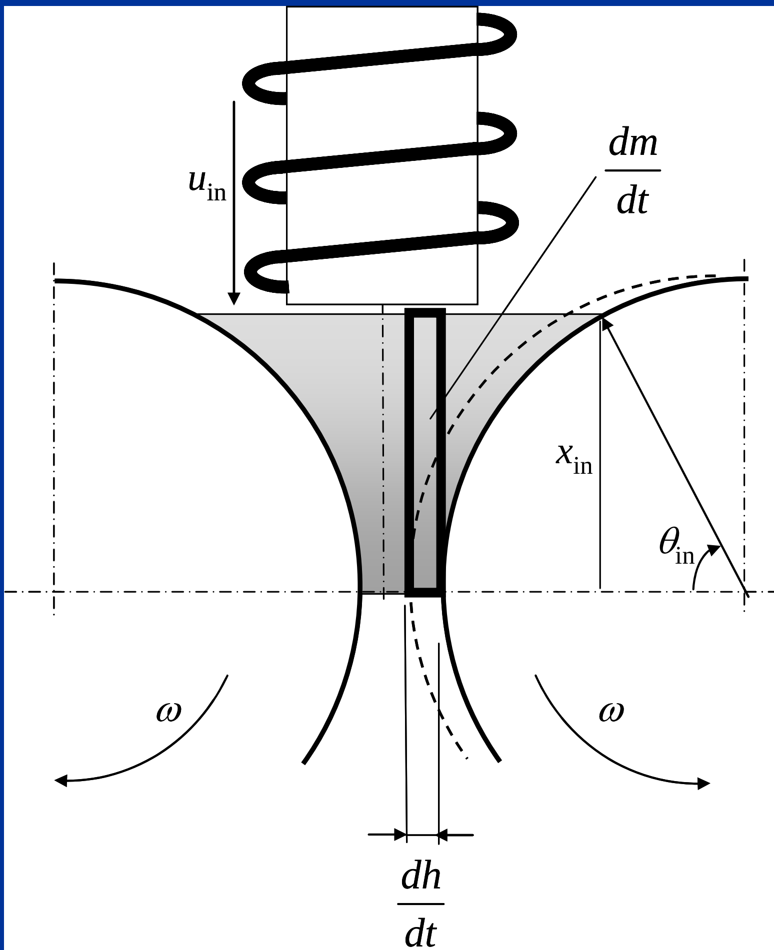
1. $h_0 \rightarrow \alpha$
2. $F, h_0, \alpha \rightarrow \sigma_{\text{exit}} \rightarrow \rho_{\text{exit}}$

Johanson's Rolling Theory(Cont'd)



- Limitations
  - No time dependency
    - Predict steady state behaviors
    - Not suitable for the control purpose
  - The effects of roll speed and feed speed are not considered at all

Material Balance



$$\frac{dm}{dt} = \dot{m}_{in} - \dot{m}_{out}$$

$$= \rho_{in} u_{in} W (h_0 + R - R\cos\theta_{in}) - \rho_{exit} R \omega W$$

$$\Delta m = \left[\int_0^{x_{in}} \rho dx \right] W \Delta h$$

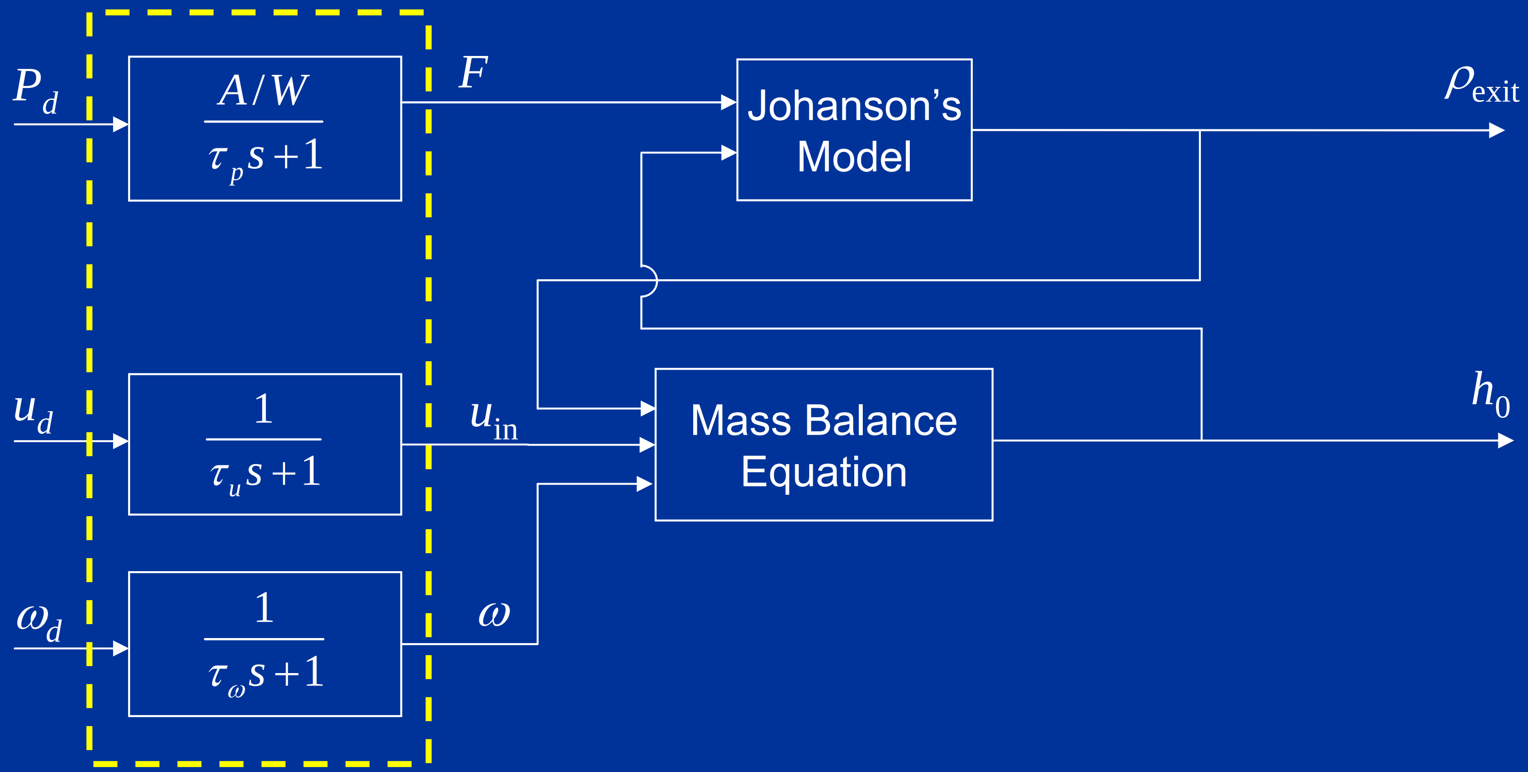
$$\frac{d}{dt}\left(\frac{h_0}{R}\right) = \frac{\omega \left[\rho_{in} \cos\theta_{in} \left(\frac{u_{in}}{\omega R}\right)\left(\frac{h_0}{R} + 1 - \cos\theta_{in}\right) - \rho_{exit}\left(\frac{h_0}{R}\right)\right]}{\int_0^{\theta_{in}} \rho(\theta)\cos\theta d\theta}$$

$$\int_0^{\theta_{in}} \rho(\theta)\cos\theta d\theta = \rho_{exit}\left(\frac{h_0}{R}\right)\left\{ \frac{2\left(1+\frac{h_0}{R}\right)}{\sqrt{\frac{h_0}{R}\left(2+\frac{h_0}{R}\right)}} \tan^{-1}\left[\sqrt{1+\frac{2R}{h_0}}\tan\frac{\alpha}{2}\right] - \alpha \right\} + \rho_{in}\left(\cos\nu - \sin\alpha\right)$$

Assumptions:

- The density in the slip region does not change
- The density change in the release region is negligible

Process Simulation



- Actuator dynamics
  - Approximated by first order dynamic models with different time constants

Process Simulation (Cont'd)

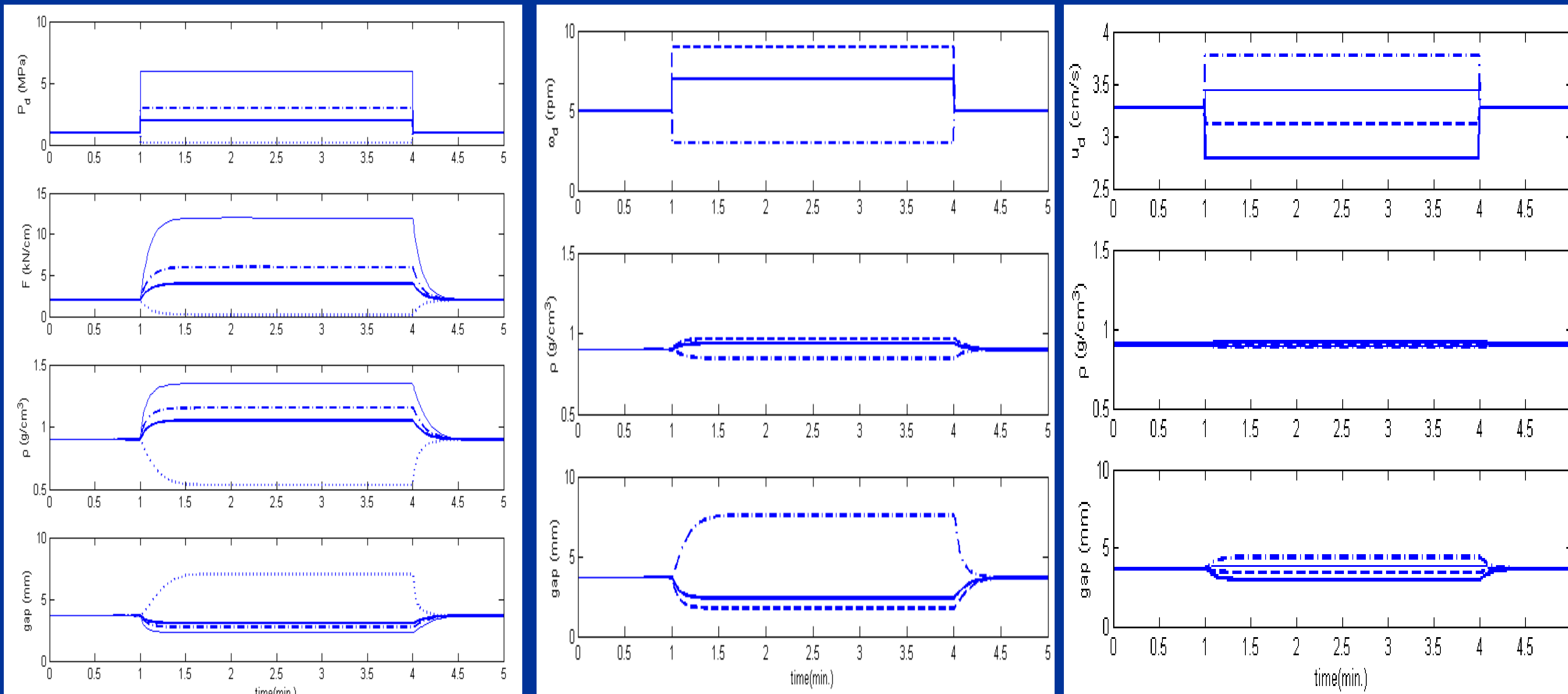
- Material
  - Microcrystalline cellulose grade Avicel PH102 (FMC Biopolymer, USA)
- Operating condition
  - Roll gap = 3.66 mm
  - Ribbon density = 0.900 g/cm^3
  - Hydraulic pressure = 1 MPa
  - Roll speed = 5 rpm
  - Feed speed = 9.82 cm/s
  - Inlet powder density = 0.300 g/cm^3
- Understand process dynamics
  - Control system design

Process Parameters & Steady State Conditions

Symbol	Description	Value
Process parameters:		
δ	Effective angle of friction	40.5°
ϕ	Angle of wall friction	18.0°
R	Radius of the rollers	12.5 cm
A	Compact surface area	100 cm^2
W	Roll width	5 cm
τ_p	Time constant of the roll force response due to the change of hydraulic pressure	6 sec.
τ_ω	Time constant of the roll speed response	6 sec.
τ_u	Time constant of the feed speed response	6 sec.
ρ_{in}	Inlet density	0.3 g/cm^3
C_1^*	Pre-exponential coefficient in the model of material compression	7.5×10^{-8} $Pa/(kg/m^3)^{4.97}$
K^*	Compressibility factor	4.97
Steady state conditions:		
$2h_0$	Roll gap	3.66 mm
ρ_{exit}	Compact density	0.900 g/cm^3
P_d	Hydraulic pressure	1 MPa
ω_d	Roll speed	5 rpm
u_d	Feed speed	3.27 cm/sec

* Bindhumadhavan, G., Seville, J. P. K., Adams, M. J., Greenwood, R. W., and Fitzpartrick, S. (2005). "Roll compaction of a pharmaceutical excipient: experimental validation of rolling theory for granular solids." *Chemical Engineering Science*, 60, 3891-3897.

Simulation Results



- Roll pressure ↑ ⇨ribbon density ↑ , roll gap ↓
- Roll speed ↑ ⇨ ribbon density ↑, roll gap ↓
- Feed speed ↑ ⇨ ribbon density ×, roll gap ↑

- Roll pressure ↓ ⇨ roll gap ↑
- Roll speed ↓ ⇨ roll gap ↑
- Feed speed ↓ ⇨ roll gap ↓

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