The Effect of Model Parameters of the Soft-Sphere Scheme on Particle-Particle Collisions

NETL Multiphase flow Conference 2012

May 22nd -24th ,2012

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Supported by

DOE-NETL (Grant #:DE-NT0008064), and NSF

Outline

- Rationale
- The Importance of the RDPM/IBM
- Soft-Sphere Model
- How to determine k_n and η_n
- Effects on Drafting Kissing and Tumbling
- Conclusions

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Rationale

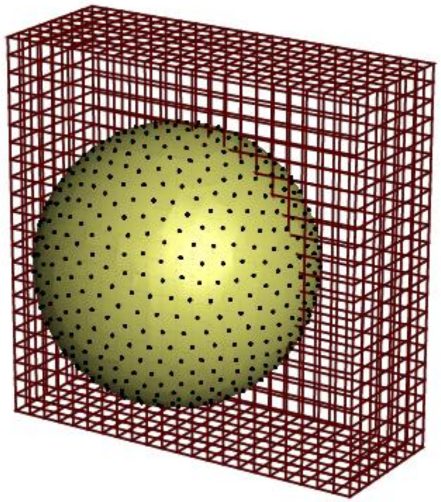
- Eulerian and Lagrangian systems need a scheme to model particle-particle or particle-wall collisions.

- The soft-sphere scheme is the most common. How do we choose the spring stiffness and damping coefficient in a soft-sphere collision model?

- How do the collision parameters affect the particle dynamics when particles collide?

Resolved Discrete Particle Method (RDPM with IBM)

- Existing collision models are:
  - Hard sphere
    - ❖event driven→ one collision at a time
  - Soft sphere
    - ❖time driven → multiple collisions at a time
  - Repulsive force
  - Lubrication force
- The Discrete particle method (DPM) a.k.a. DNS has the capability of handling particle-particle/wall collisions unlike MFIX and DEM



Fixed Eulerian grid & Moving Lagrangian

Courtesy: A combined soft-sphere collision / IBM for Resolved simulations of particulate flows Wim-Paul Breugem Laboratory for Aero & Hydrodynamics

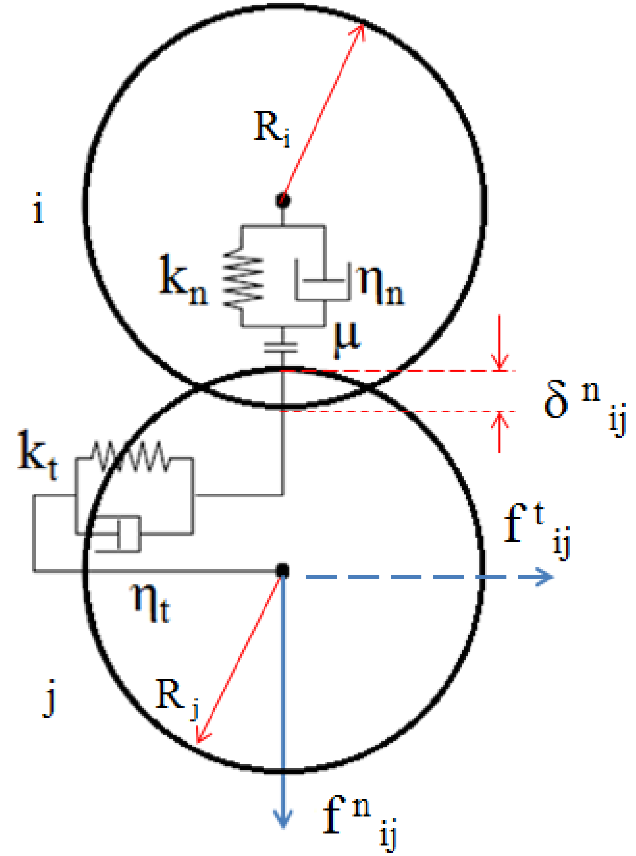
- The RPDM/IBM approach is advantageous because:
  - it effectively handles overlap
  - No regridding is required for moving particles.

Soft-Sphere collision model

- Its simplest form is the **linear spring-dashpot model**
- Allows particles to slightly **overlap** (<0.5% d).

For two particles **i** and **j** , the force balance for collisions in the normal direction is :

$$f^{n}{}_{ij} = -k_n \delta^{n}{}_{ij} - \eta_n v^{n}{}_{ij}$$



Soft-Sphere Model Parameters

δ^n_{ij} :normal overlap displacement

k_n :normal Spring Stiffness

η_n :normal damping coefficient

v^n_{ij} :normal relative velocity

$$f^n_{ij} = -k_n \delta^n_{ij} - \eta_n v^n_{ij}$$

$$v^n_{ij} = (v_{ij} \cdot n_{ij}) n_{ij}$$

The reduced mass is given as:

$$m_{ij} = \left(\frac{1}{m_i} + \frac{1}{m_j} \right)^{-1}$$

We can do same for collisions in the tangential direction

Soft-Sphere Model Parameters cont.

For dry collisions (in air) the following analytical solution is obtained ,Hoomans et al. [1]

$$\eta_n = \begin{cases} \dfrac{-2\ln(e_n)\sqrt{m_{ij}k_n}}{\sqrt{\pi^2 + \ln^2(e_n)}} & \text{if} \quad e_n \neq 0 \\ 2\sqrt{m_{ij}k_n} & \text{if} \quad e_n = 0 \end{cases}$$

e_n:the normal coefficient of restitution

η_n: in terms of k_n and e_n

the normal contact time is expressed as:

$$t_{con,n} = \sqrt{m_{ij}\frac{\pi^2 + \ln^2(e_n)}{k_n}} = N_c\delta t$$

N_c : the number of computational time steps with $N_c > 1$

δt : time step with $\delta t < t_{con,n}$

[1] Hoomans et al.2000. Granular dynamics simulation of segregation phenomena ... Powder Technology 109 (1–3), 41–48.

Soft Sphere Collision Parameters N_c and e_n

$$k_n = m_{ij} \frac{\pi^2 + \ln^2(e_n)}{(N_c \delta t)^2}$$

$$\eta_n = -\frac{2 m_{ij} \ln(e_n)}{N_c \delta t}$$

In dry collisions the contact force dominates the drag force and so can be neglected

dry collisions can be used to approximate collisions in a viscous fluid

N_c and e_n are now the inputs that link η_n and k_n

How to determine k_n and η_n for a collision process

- Experimental methods, Muller et al. [2]

  k_n=3x10^5~10^6 dyn/cm

  - gives a very wide range of results for $\mathbf{k_n}$
  - Uses $\mathbf{k_n}$ and $\mathbf{e_n}$ graphically to find $\boldsymbol{\eta_n}$
- Trial and Error methods, Xu and Yu [3]
  - less elegant

- Method being introduced:

  Using N_c and e_n with δt given to find $\mathbf{k_n}$ and $\boldsymbol{\eta_n}$

  - (more elegant)

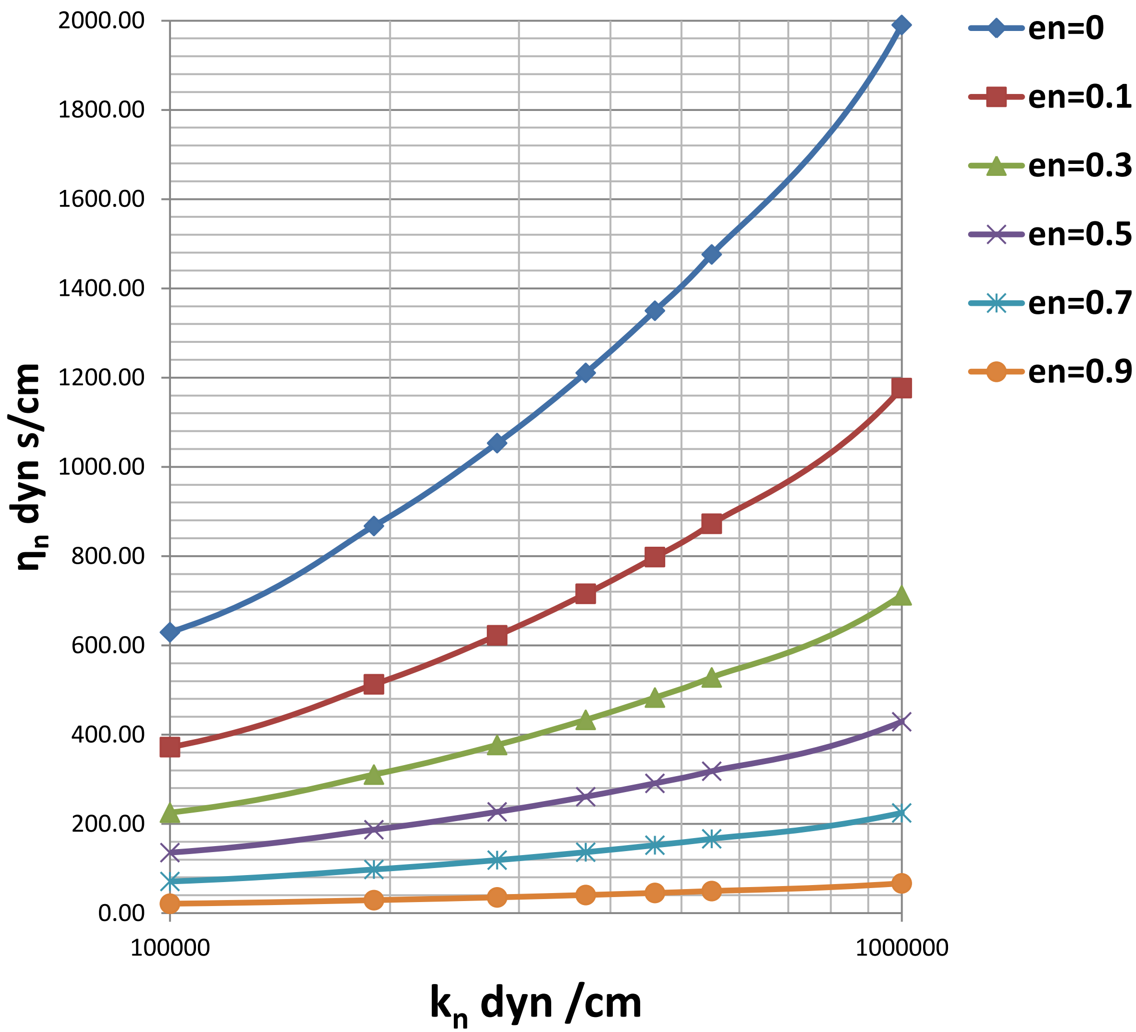
[2] Mullier et al., 1991, "A Single-Particle Friction Cell for… Granular Materials," Powder Technol., 65, pp. 61–74.
[3] Xu, B.H. and Yu, A.B., (1997). Numerical simulation of the gas-solid flow in a fluidized… Chem.Engng Sci. 52, 2785.

Experimental/Graphical Approach

k_n	$\eta_n(e_n=0)$	$\eta_n(e_n=0.8)$	$t_{cont,n}$	N_c		
dyn/cm	dyn s/cm	dyn s/cm	s	δt=0.25E-3	δt=0.5E-3	δt=1E-3
100	19.90	1.41	0.3134	1254	626.82	313.41
1000	62.94	4.46	0.0991	396	198.22	99.11
5000	140.73	9.97	0.0443	177	88.65	44.32
50000	445.03	31.53	0.0140	56	28.03	14.02
100000	629.36	44.59	0.0099	40	19.82	9.91
500000	1407.30	99.71	0.0044	18	8.86	4.43
1000000	1990.22	141.01	0.0031	13	6.27	3.13
10000000	6293.64	445.91	0.0010	4	1.98	0.99

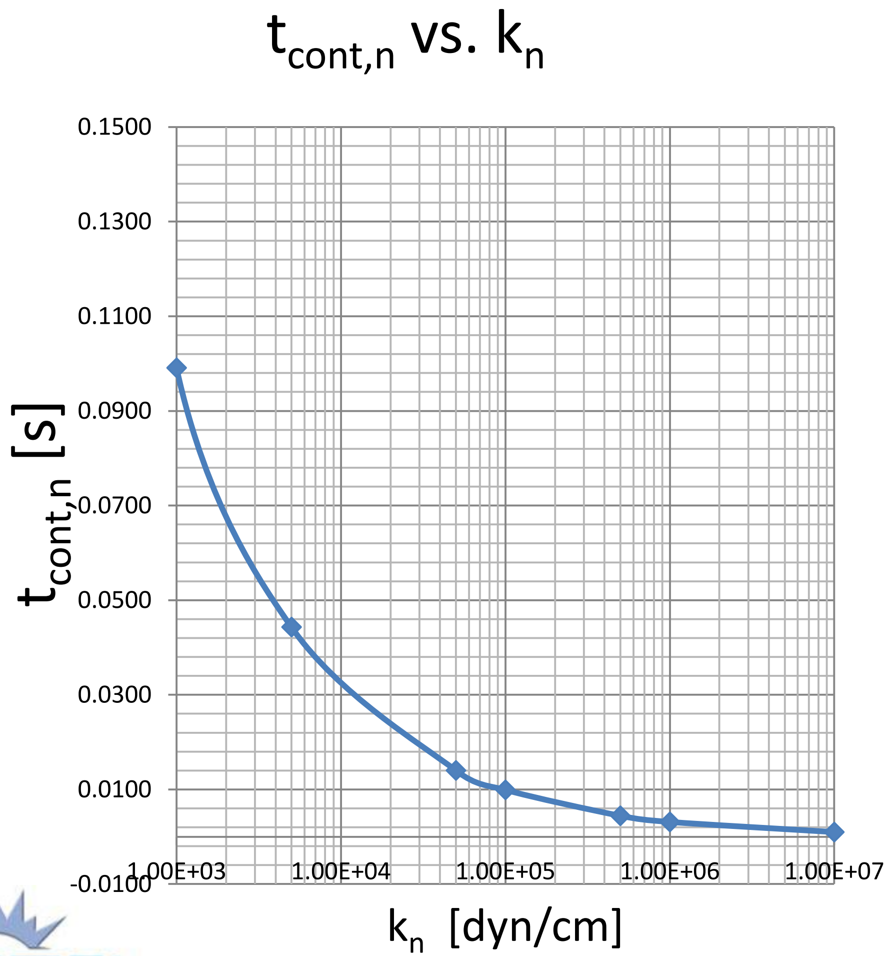
Finding η_n from k_n , e_n

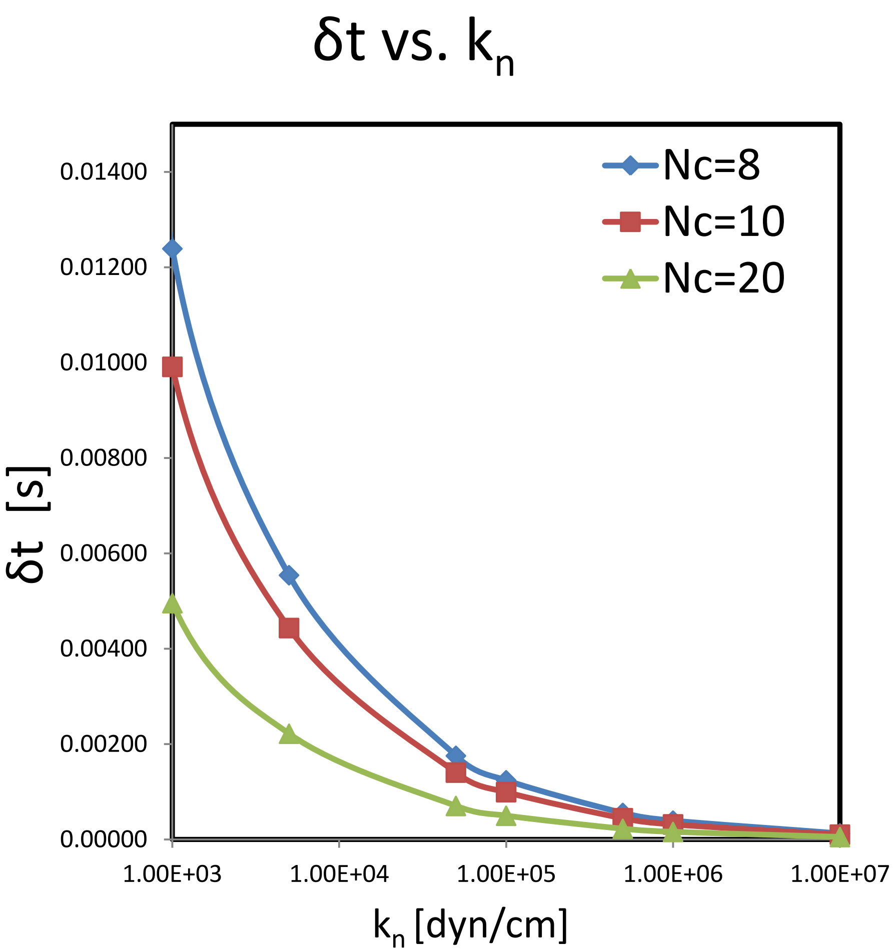
η_n is obtained graphically from k_n and e_n (0 ~ 0.9)



The range of k_n that is of interest is (10^5 ~ 10^6) dyn/cm

Relationship between δt and k_n





Finding η_n and k_n from Nc, e_n

1. Predictions from the **<u>non-linear</u>** **Hertz contact theory** are used to get the **lower limit** of the contact time **($N_c\delta t$ ~ 10^{-9}s)**

$$K = \frac{8E}{15(1-\sigma^2)}\sqrt{\frac{R_i R_j}{R_i + R_j}} \qquad t_{con,n} = 2.94\left[\frac{m_{ij}}{K^2 v^n{}_{ij}}\right]^{\frac{1}{5}} = N_c\delta t$$

E is the Young's modulus and **σ** is the Poisson's ratio

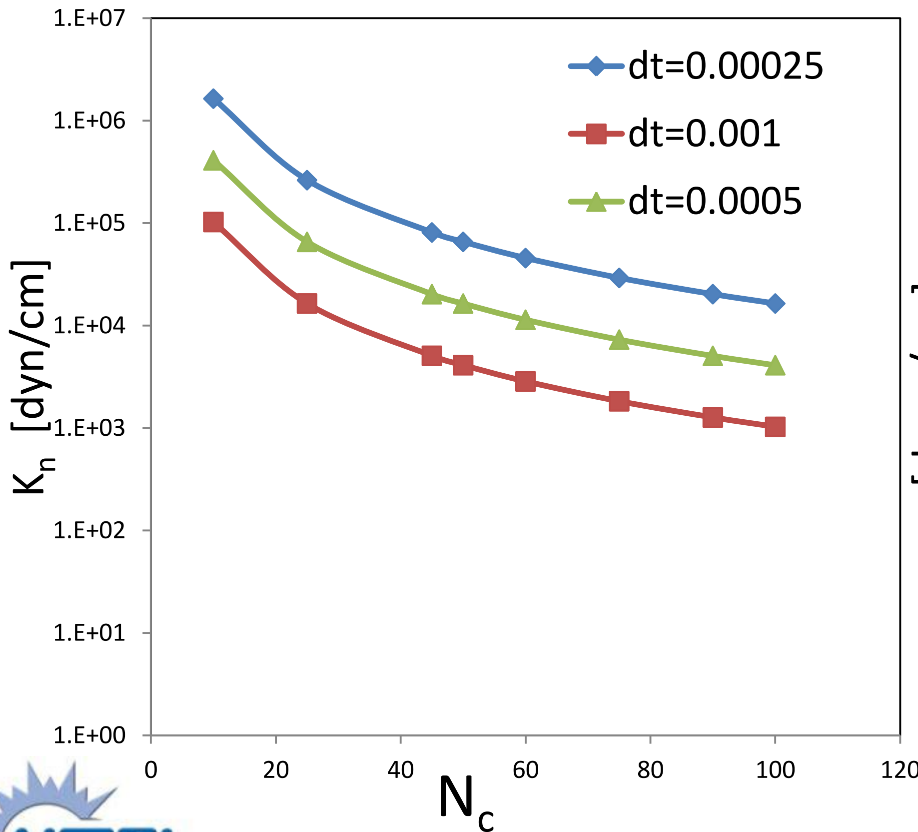
2. From the discussion of **Van der Hoef et al. [4]**
   - Choose **($N_c\delta t$)** **<u>not too large</u>** to allow severe overlapping between particles
   - Choose **($N_c\delta t$)** **<u>not too small</u>** to accurately resolve collision in time (inaccuracy)

First, we use stability/convergence tests to find a value for **δt**
We vary **N_c** to find a range that satisfies the above limits

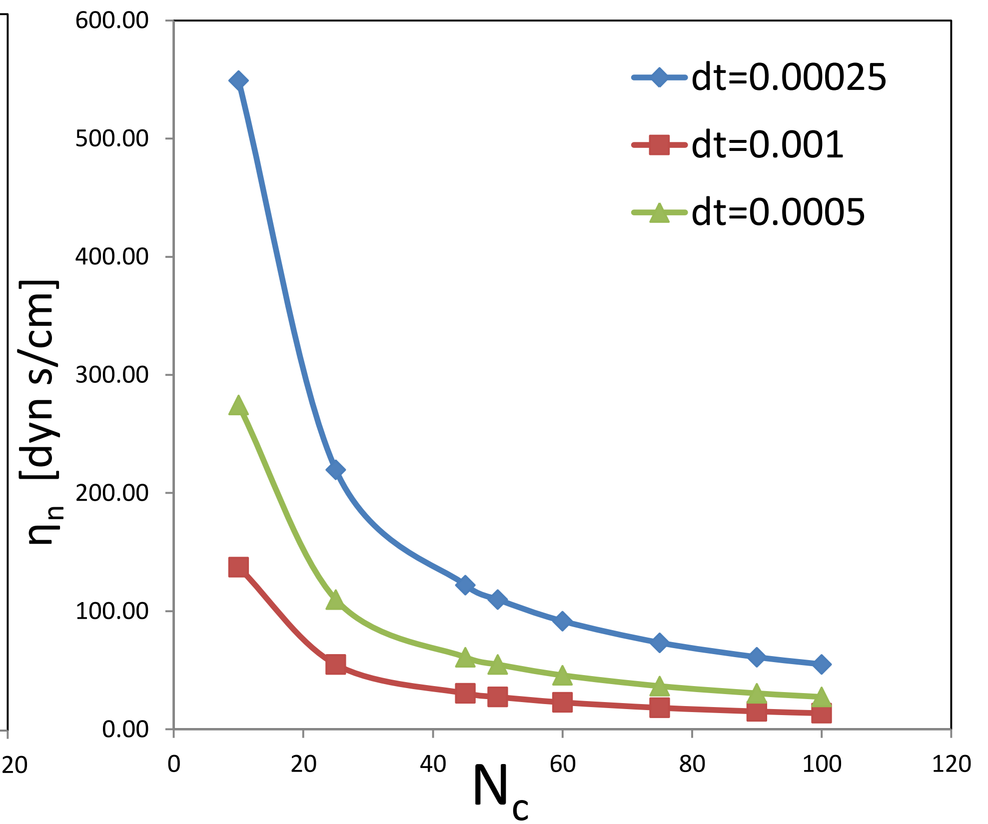
[4] Van der Hoef et al.2006. Multi-scale modeling of gas-fuidized beds.. Adv.Chem. Engng, 31, pp. 65.149.

Relationship between η_n / k_n and N_c for different time steps

k_n vs N_c



η_n vs N_c



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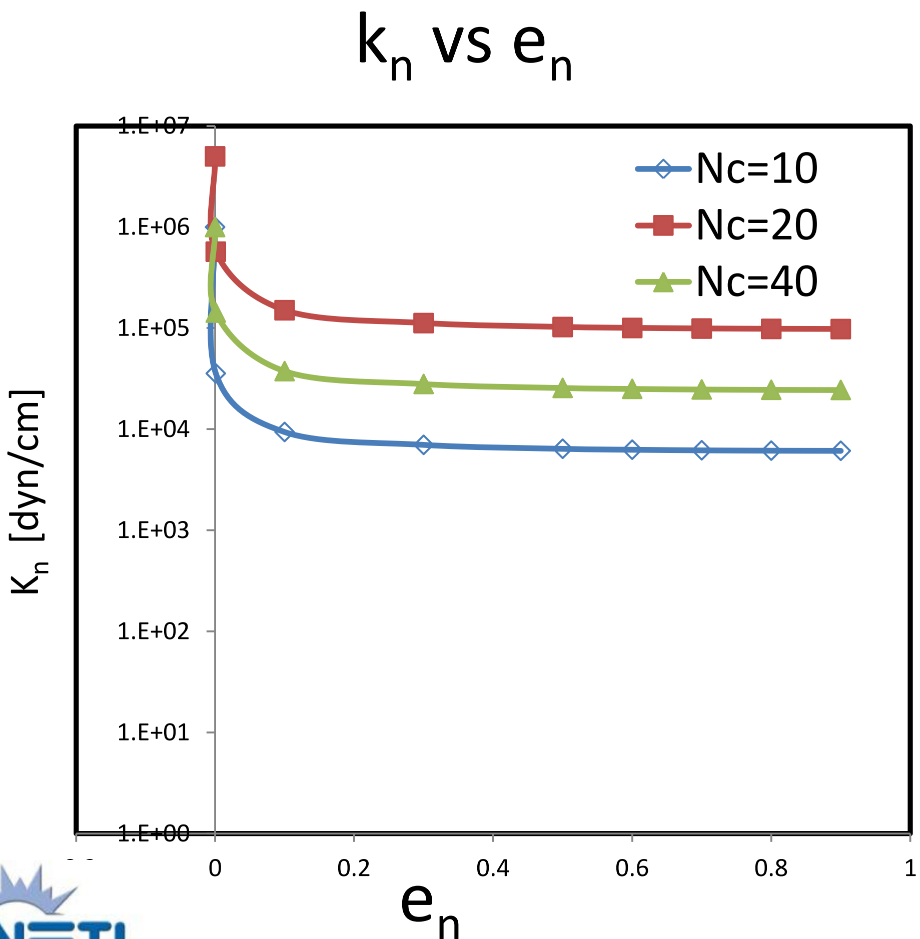
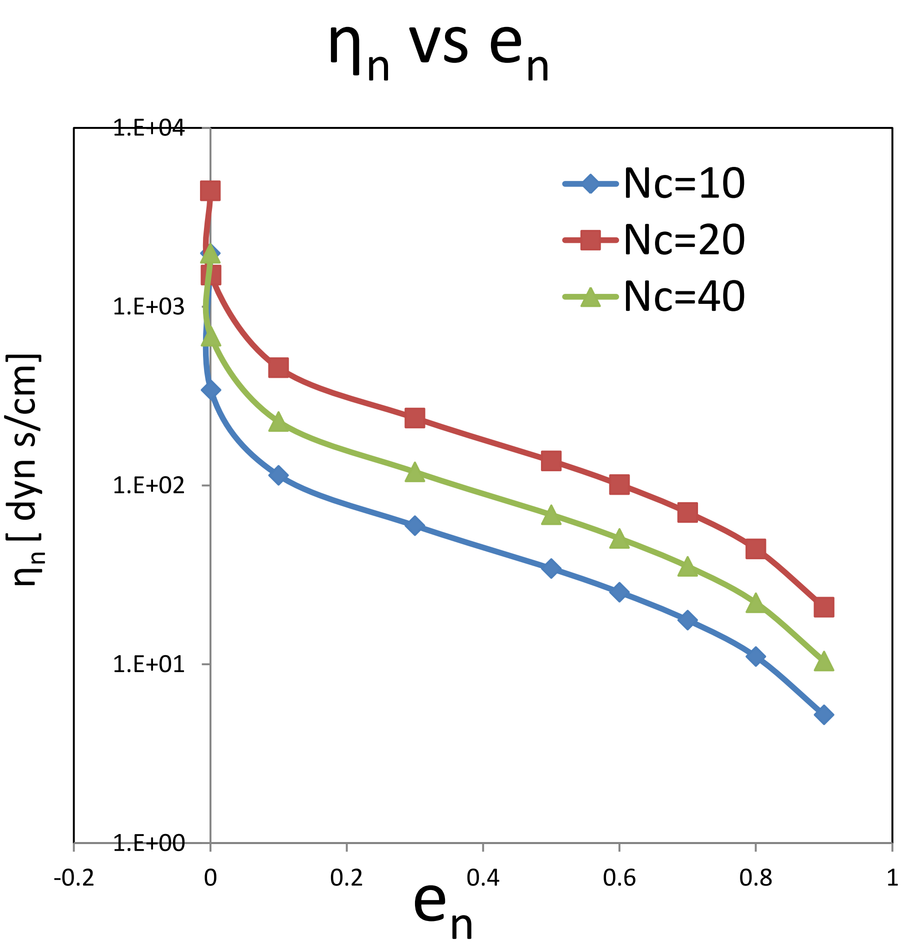
Relationship between η_n /k_n and e_n for different Nc's



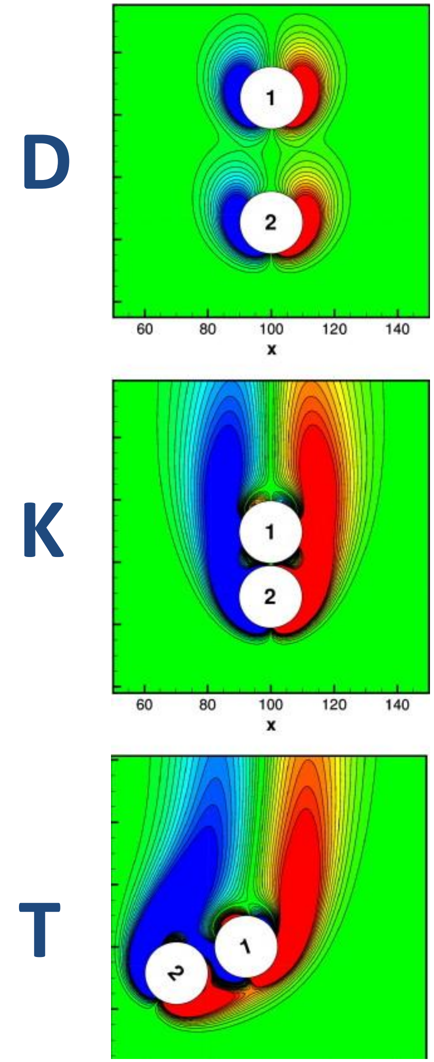


Effects of the Collision scheme on Drafting Kissing and Tumbling (DKT)

What is DKT ?

During Sedimentation
particles experience DKT

- Drafting ⇒Attraction due to low pressure
- Kissing ⇒ Repeated collisions
- Tumbling ⇒ Rolling on each other



Courtesy: *International Journal of Multiphase Flow Volume 35, Issue 9, September 2009, Pages 854–867*

Effect of Collision Parameters on DKT

To study k_n and DKT we use:

k_n =1000, $5x10^4$, $5x10^5$ dyn/cm

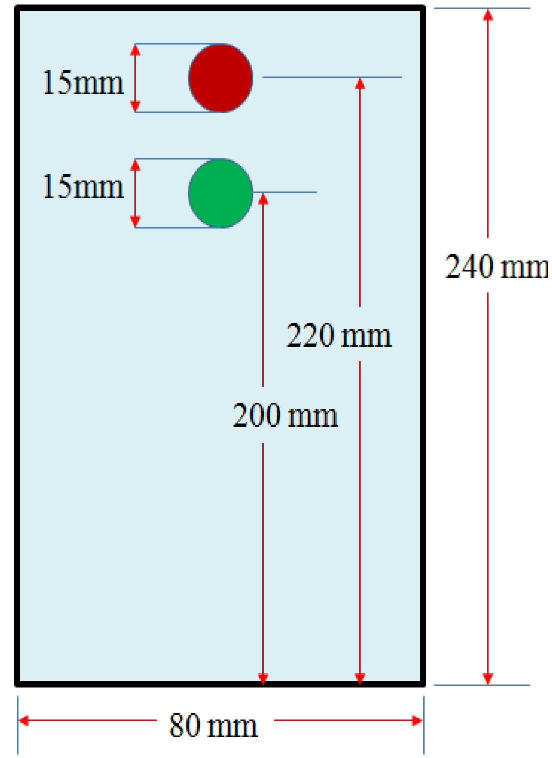
η_n =100 dyn s/cm

To study η_n and DKT we use :

η_n =0, 50 , 100 dyn s/cm

k_n=50000 dyn /cm

The results show that as k_n and η_n decrease the softer the collisions get and the longer the kissing process



ρ_p=1120 kg/m3

ρ_f =962 kg/m3

μ = 0.913Ns/m2

d_p=15 mm

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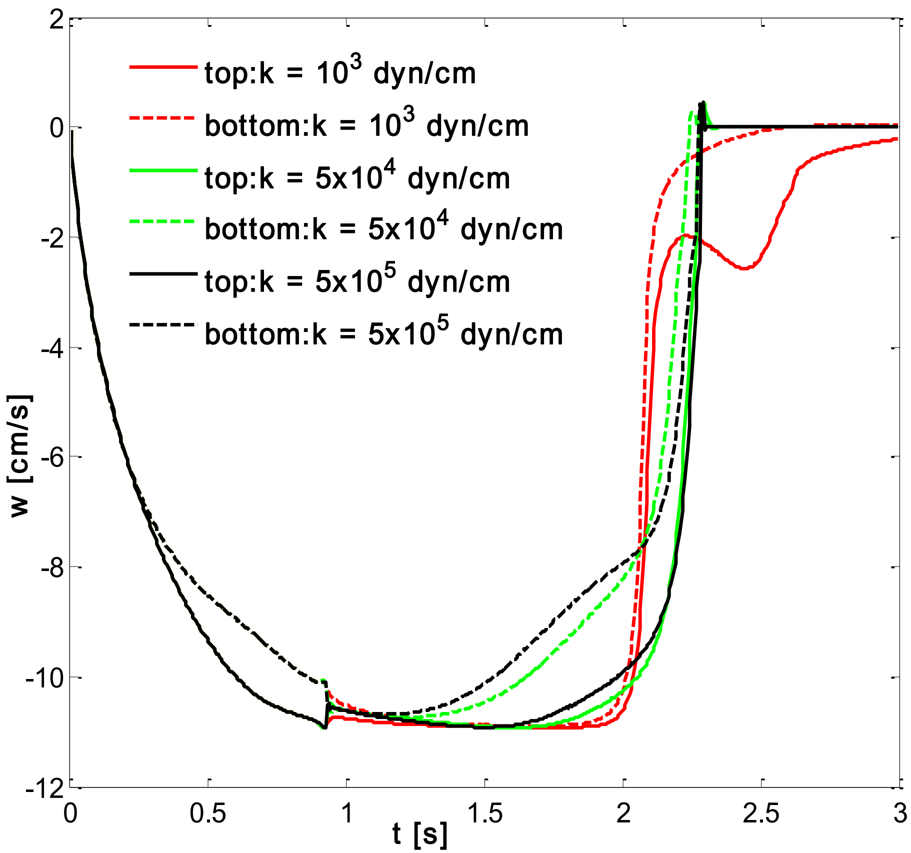
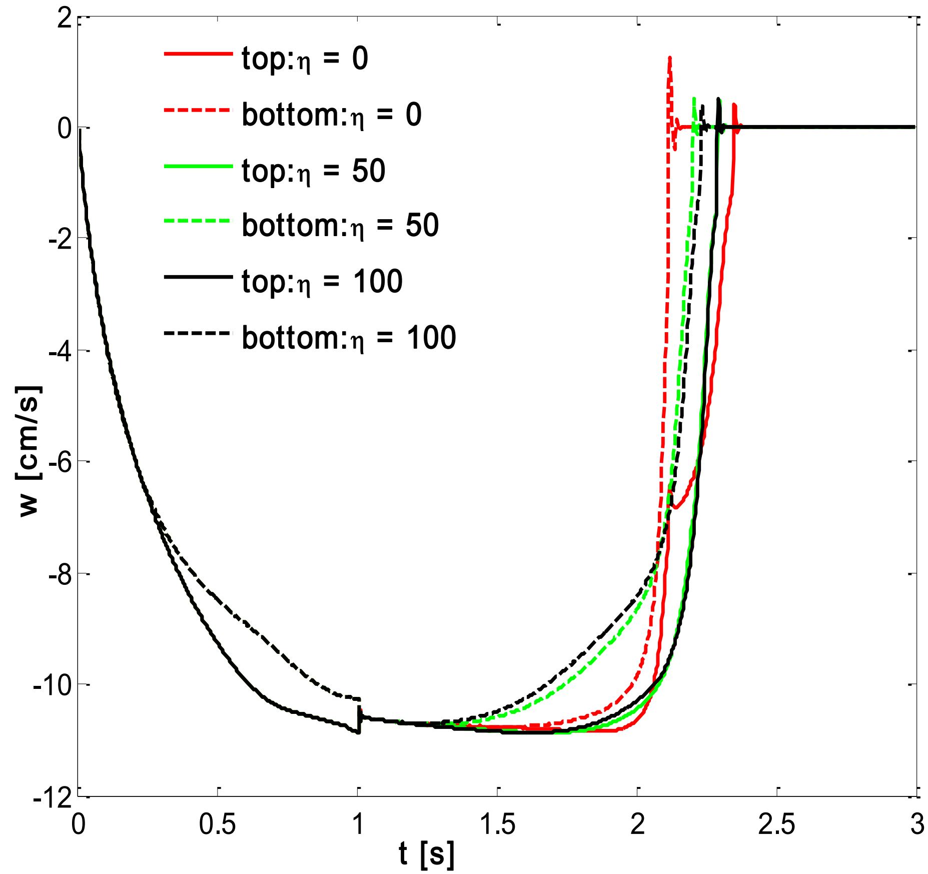
Results:Settling velocity and DKT



Particle settling velocity for different k_n



Particle settling velocity for different η_n

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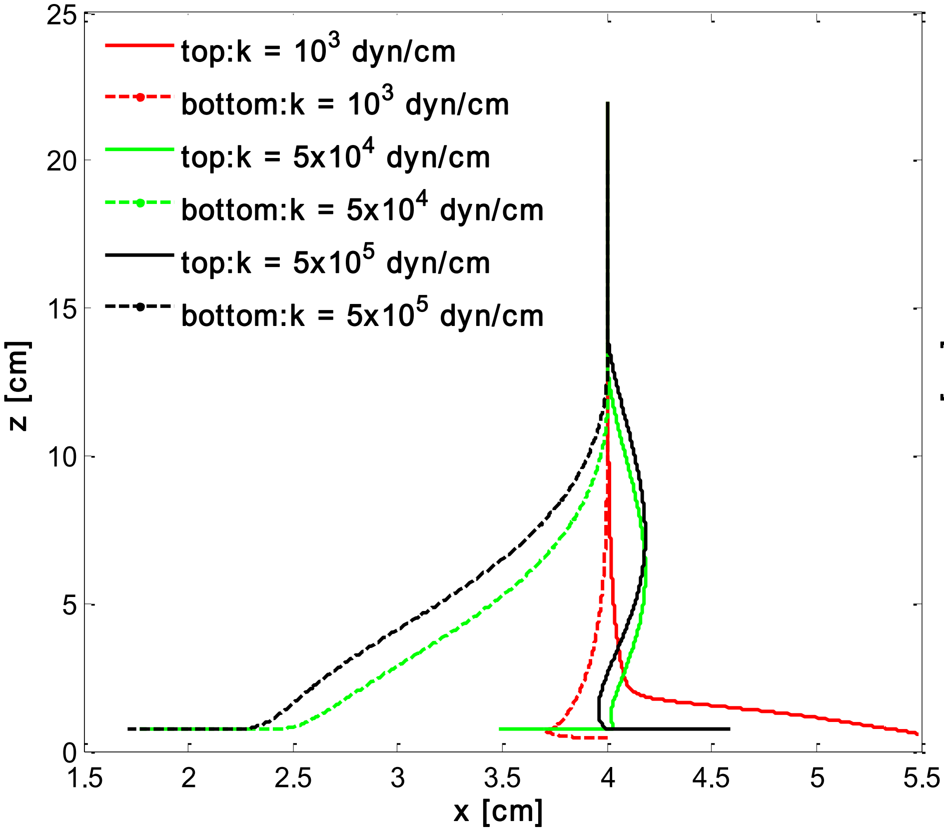
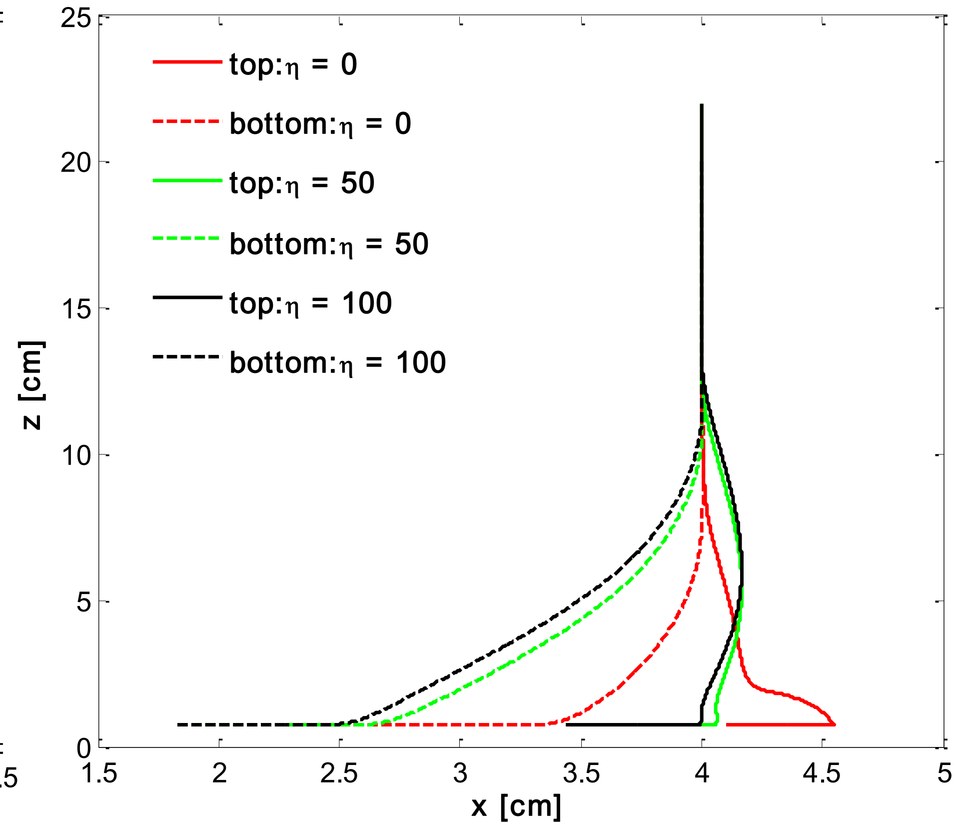
Results:Settling Trajectory and DKT



Particle settling trajectory at different k_n



Particle settling trajectory for different η_n

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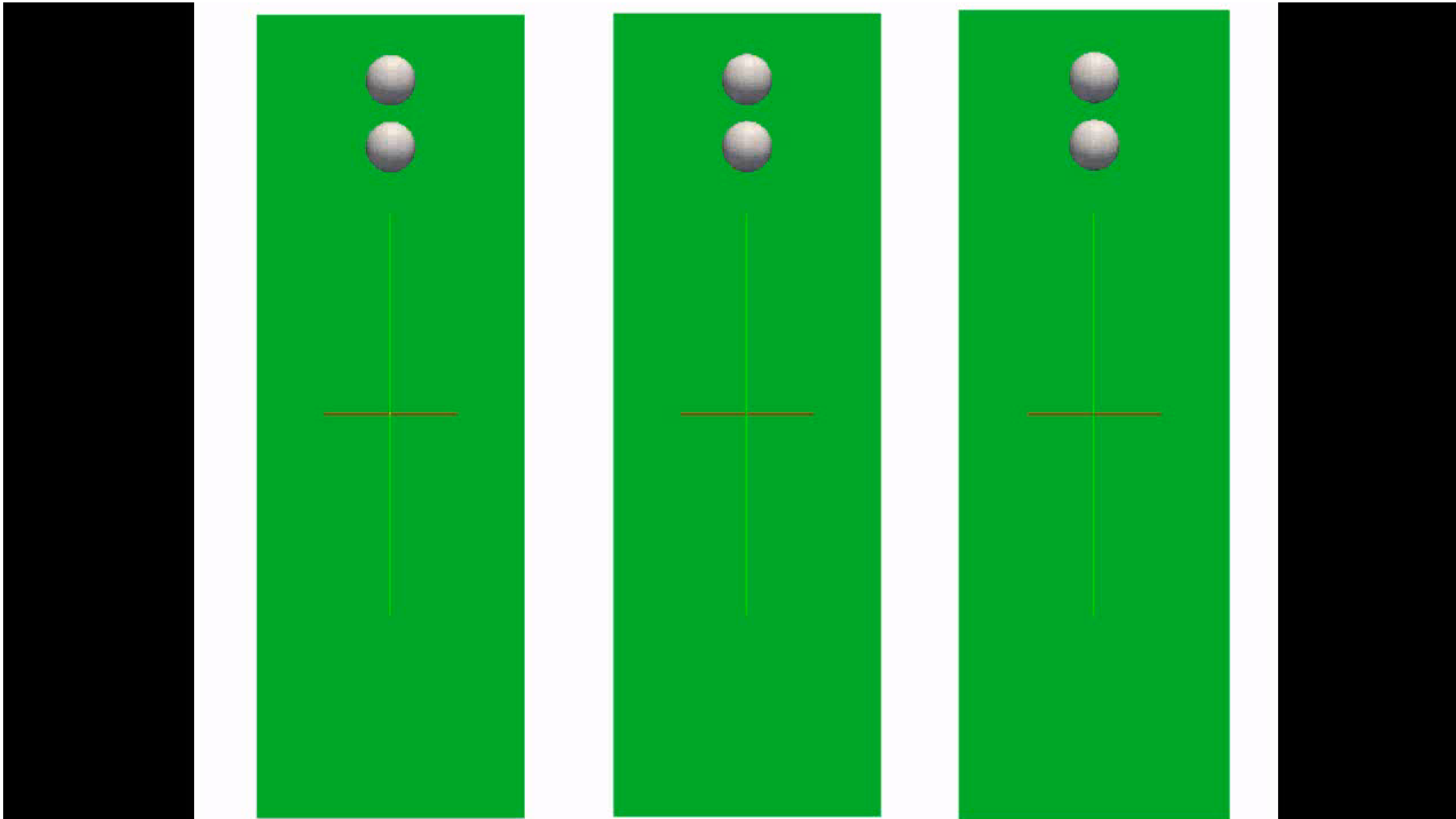
Spring Stiffness and DKT-video

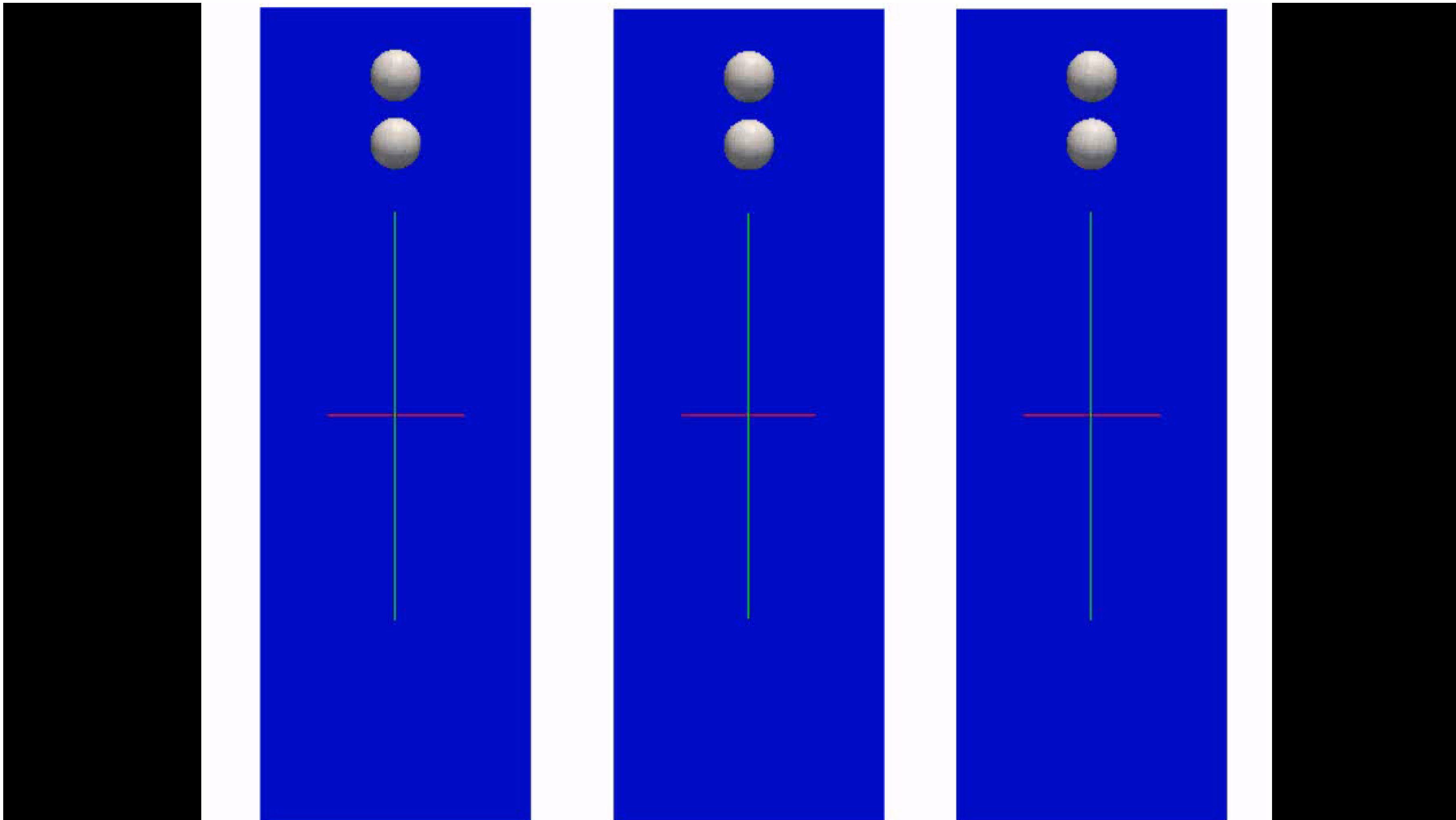


k_n =1000

k_n =50000

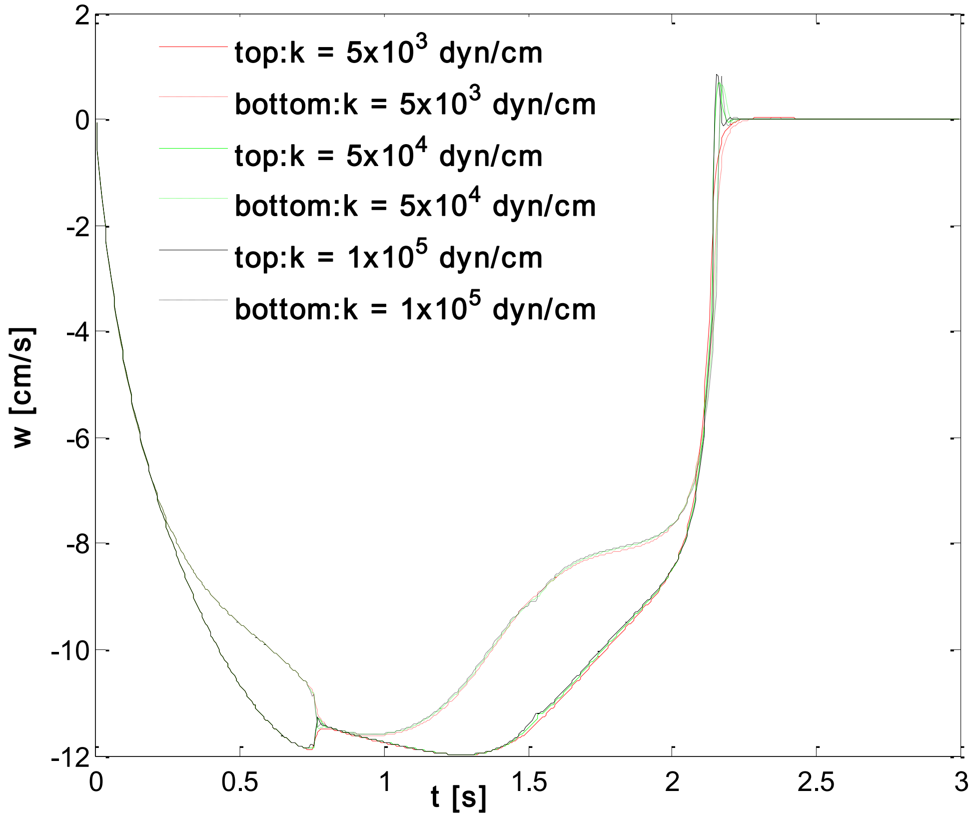
k_n=500000

Damping Coefficient and DKT-video



η_n=0 η_n=50 η_n=100

Refining the range of k_n



Particle settling velocity for $5000 \leq k_n \leq 100{,}000$

We could by trial and error find the range: $5000 \leq k_n \leq 10^5$ dyn /cm for $\eta_n = 150$ dyn s/cm

The change in DKT with k_n was insignificant

Overlap and Contact time in DKT: refining range with N_c

Periodic kissing increases with k_n
For very small N_c (large k_n) the model approaches a hard sphere scheme with no overlap

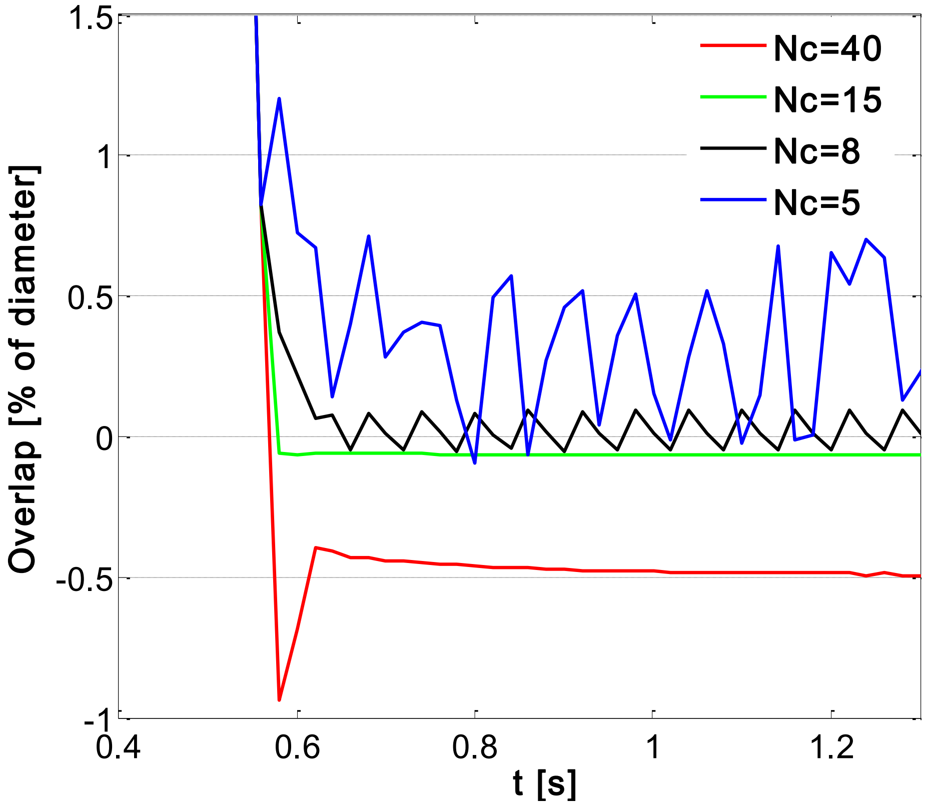
The choice of N_c is in the range:

$8 < N_c < 15$ since for this range

Overlap= %diameter < 0.5% of diameter

N_c	k_n	η_n
8	160142.35	171.60
10	102491.10	137.28
12	71174.37	114.39

Gap width [% diameter] vs time



There is a great degree of agreement with the range that was used in trial and error: $5000 \leq k_n \leq 10^5$ dyn/cm for $\eta_n = 150$ dyn s/cm

Conclusions

- k_n and η_n decrease with the time step δt
- Increasing k_n (decreasing N_c) increases the kissing process
- A graphical approach gives a foreknowledge of the range without experiments
- Two main approaches to choose the soft-sphere collision parameters:
  1. given k_n and e_n to find N_c and δt
  2. given δt we can use N_c to find k_n and η_n

     which is more elegant

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Questions?