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Developing Hydroalcoholic Gels

For the hand sanitizer market in response to shortages created during the COVID-19 pandemic – the science

Celluforce Inc.

TAPPI Nano 2021 Virtual Conference
15-16 June 2021

TAPPI NANO DIVISION

COVID-19 and Hand Sanitizer

- The sudden outbreak of Covid-19 created unprecedented demand for hand sanitizers
- Carbopol®, a key thickening agent to form hydroalcoholic gels was in severe shortage

Major Ingredients in Hand Sanitizers:

- *Alcohol (ethyl or isopropyl alcohol)*
- *Water*
- *Rheology modifier*
- *Neutralizer*
- *Emollient*

What Makes a Good Gel Hand Sanitizer

- ❑ Sanitizes
- ❑ Easy to dispense
- ❑ Has body
- ❑ Spreads smoothly
- ❑ Covers well
- ❑ Emolliates
- ❑ Cost effective
- ❑ Sustainable

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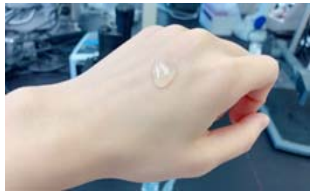
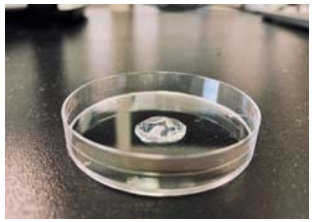
Celluforce NCC® as a Gelling Agent in Hydroalcoholic Gels





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List of alternative rheology modifiers for use in the production of hand sanitizers

Many ingredients can be considered as replacements for a rheology modifier used in a clear gel (e.g. a hydroalcoholic gel hand sanitizer). The list below contains examples of replacement rheology modifiers which can be used to form a clear or slightly hazed gel (please verify with each supplier); other ingredients may also be commercially available:

Expand all | Collapse all

Recent technologies can also be considered:

▼ Microcrystalline cellulose

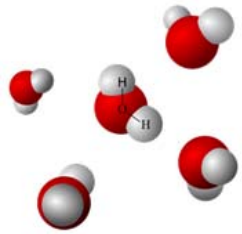
Chemical substance: Microcrystalline cellulose

- Celluforce NCC
- Exilva-FM-02-L
- Exilva-FM-02-V
- Exilva-F01-V
- Exilva-P01-V

CNC - Hand Sanitizers: The Ingredients !

1

Water



Below 36% w/w

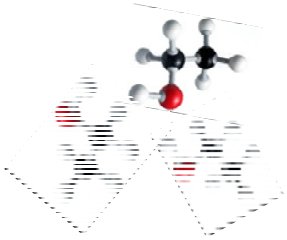
2

Cellulose Nanocrystals

1 – 2% w/w

3

Alcohol



Above 62% w/w
(70% v/v) Ethanol

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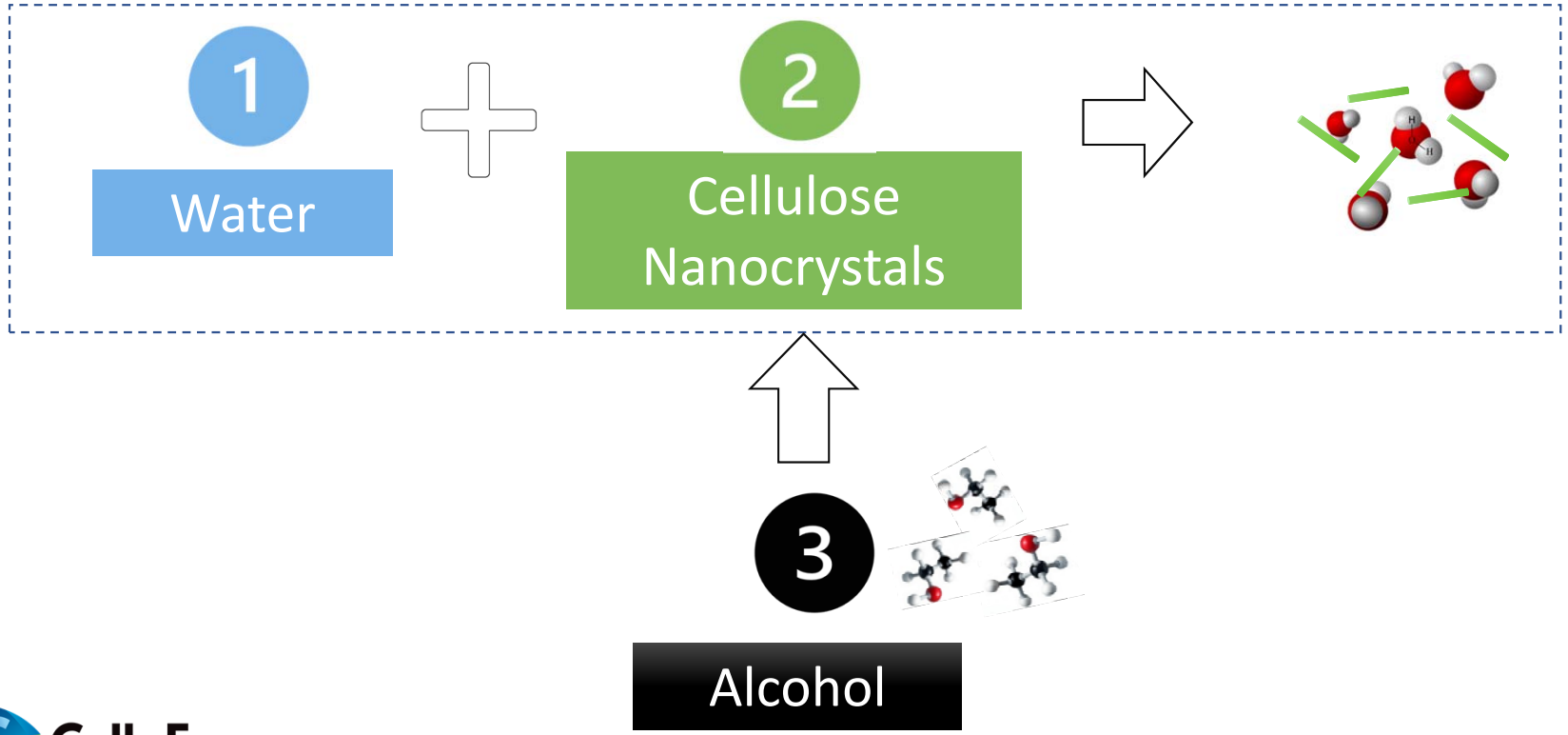
CNC - Hand Sanitizers: The Preparation !



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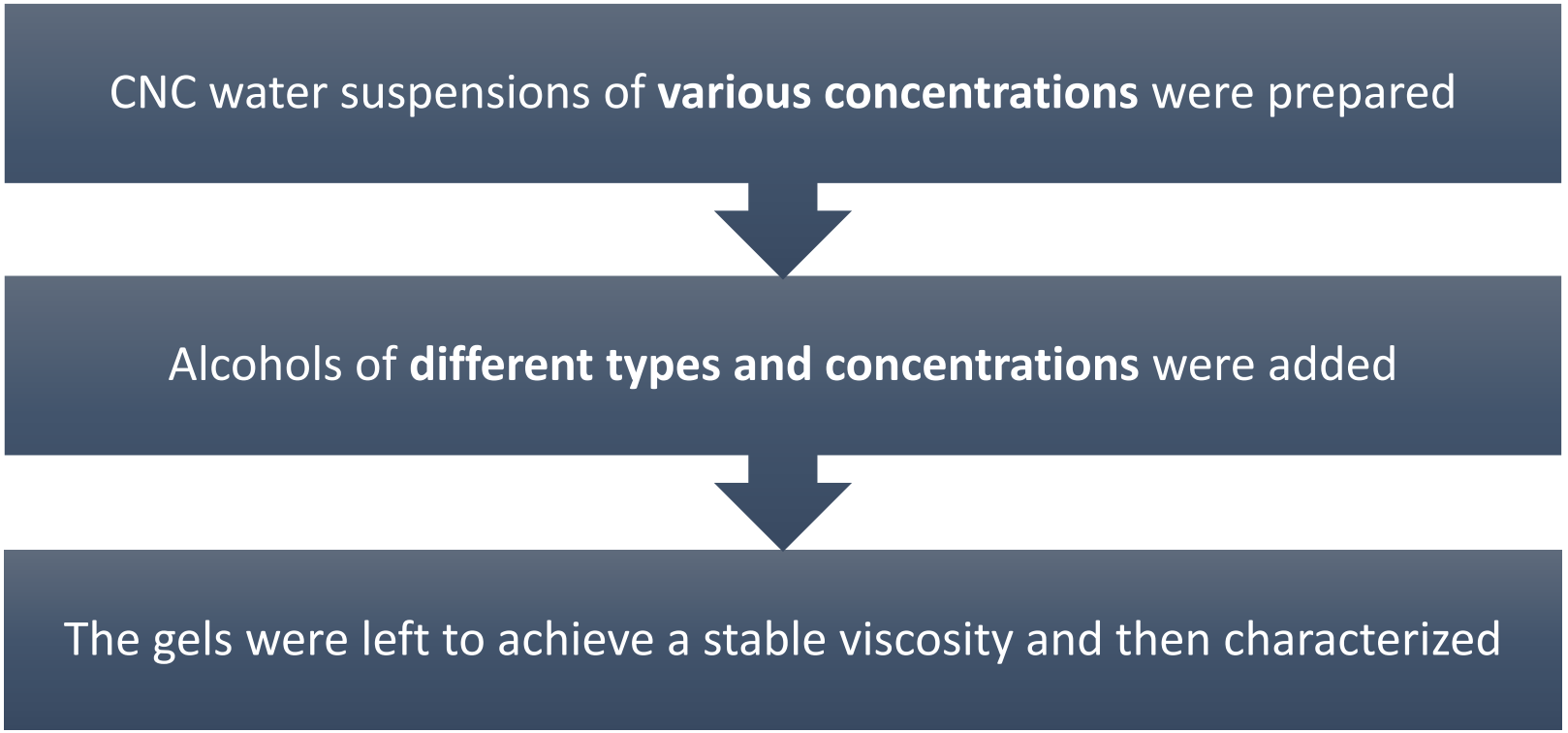
CNC-HAGs: Understanding the Science



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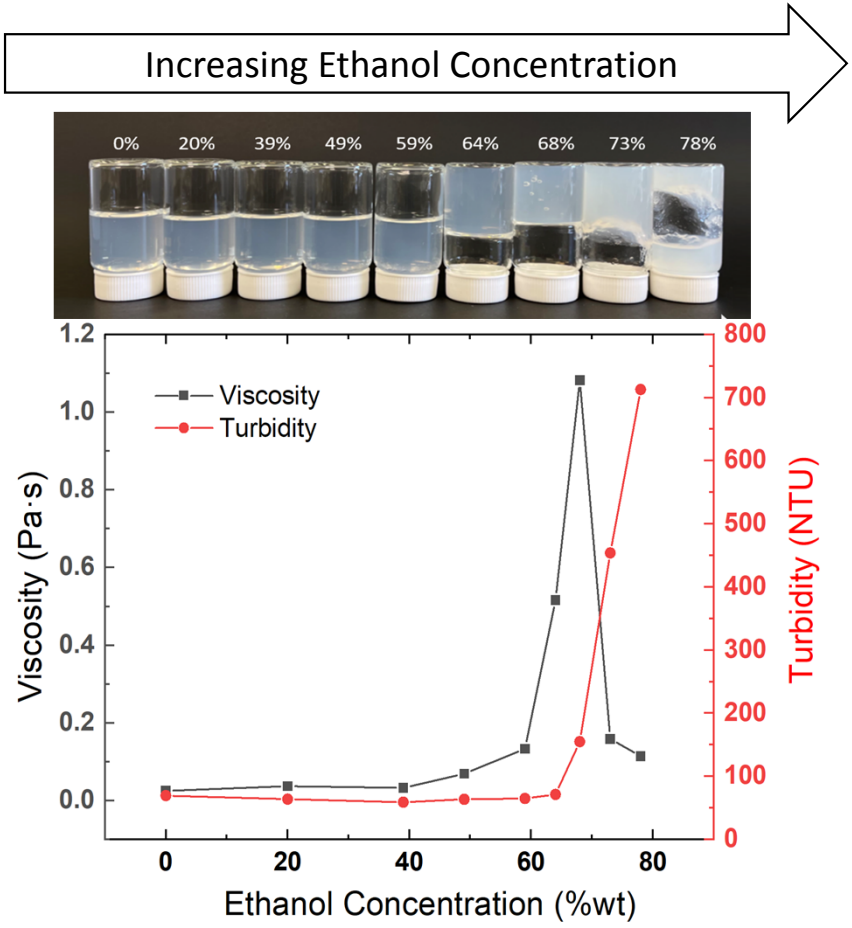
Impact of Ethanol Concentration on Gelation

- Viscosity increases steeply beyond C_{ETOH}=59%
- The transparency of the suspension remains high until C_{ETOH} = 68% (maximum viscosity)
- Both transparency and viscosity decrease sharply above C_{ETOH} = 68%



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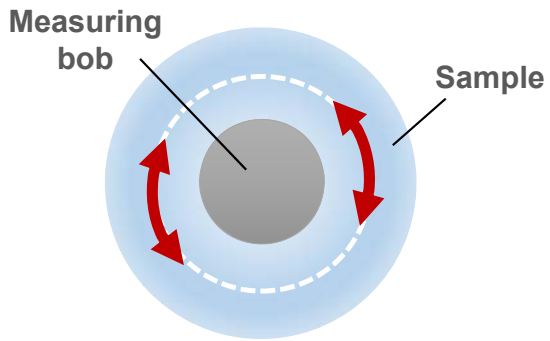
Impact of Ethanol Concentration on the Viscoelastic Behavior of HAGs

Illustration of the rotational oscillation of the measuring bob in the sample (Top-down view)



- Rheometry was used to follow the viscoelastic properties of various HAG samples
  - **Storage modulus G':**

    The ability to store deformation energy (Elasticity)
  - **Loss modulus G'':**

    The ability to dissipate deformation energy (Flowability)

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Impact of Ethanol Concentration on Viscoelastic Behavior of HAGs

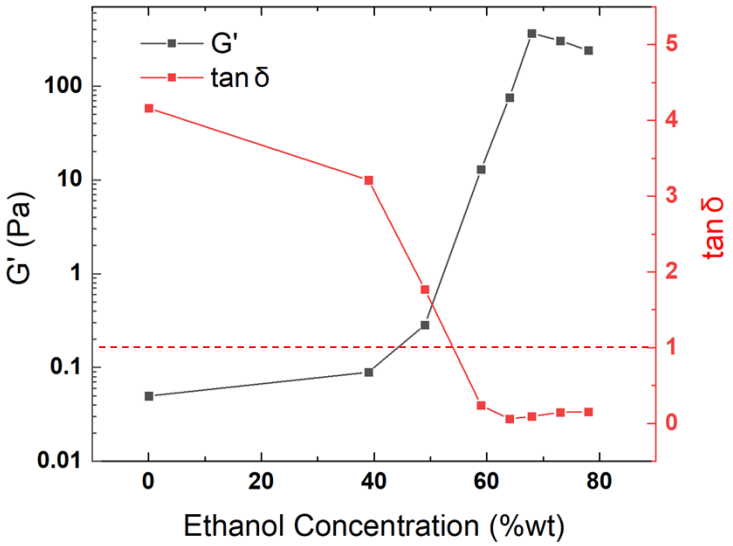
Water:
low G′, high G′′

Jello
High G′, low G′′

Tan δ = G′′/G′

- Tan δ > 1: inelastic deformation *(liquid-like behavior)*
- Tan δ < 1: elastic deformation *(solid-like behavior)*

- G′ shows a sudden increase beyond C_{ETOH} = 59% (stronger resistance to deformation indicating gelation)
- The Tan δ value also suggests that the gelation transition occurs around C_{ETOH}=59%



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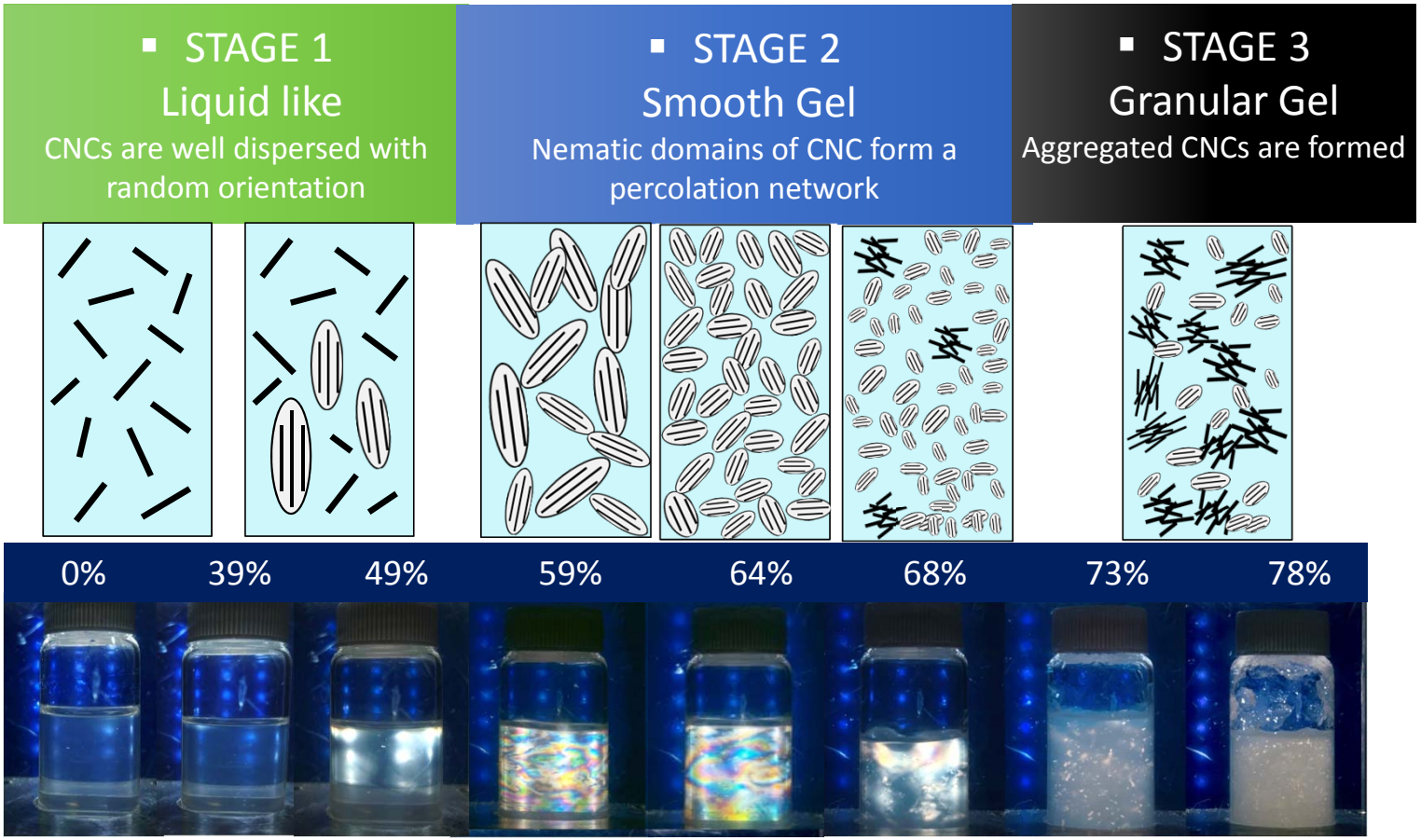
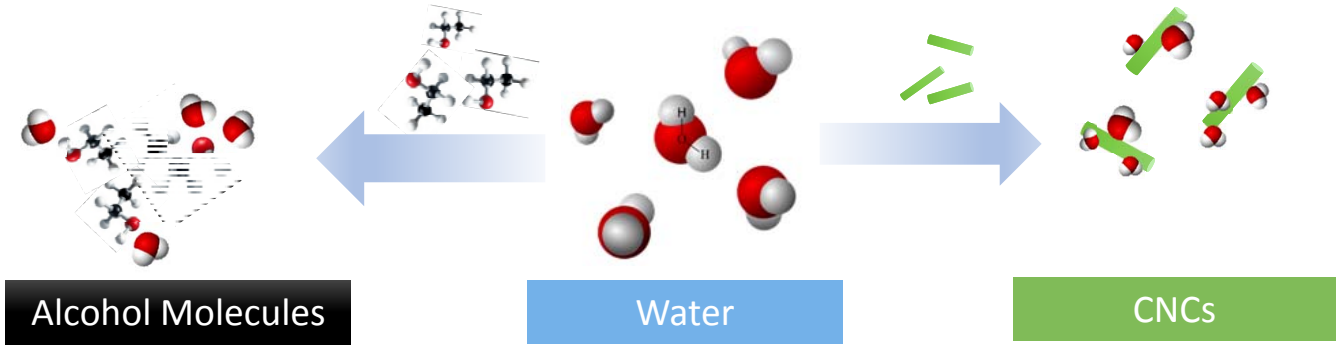
Impact of Ethanol Concentration on the CNC Dispersion



Hypothesis:
Water-Depletion-Induced Gelation

- Ethanol molecules form clusters and require water molecules to hydrate and stabilize
- CNC particles also require water molecules to stabilize
- Gelation occurs when CNCs are forced to form into a percolation network in the limited water region



Supporting Evidence:
Water and Alcohol Do Not Mix at the Molecular Level

- When alcohol is mixed with water, the entropy increases far less than it would in a well-mixed system
- Alcohol molecules form microscale hydrophobic environments due to preferential self-association into clusters
- Alcohol clusters are stabilized by hydrogen bonding with surrounding water at the interfaces

nature

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Published: 25 April 2002

Molecular segregation observed in a concentrated alcohol–water solution

S. Dixit, J. Crain, W. C. K. Poon, J. L. Finney & A. K. Soper

Nature **416**, 829–832(2002) | Cite this article

1819 Accesses | **746** Citations | **17** Altmetric | Metrics

ELSEVIER

Journal of Molecular Liquids

Volume 90, Issues 1–3, February 2001, Pages 175-184

Solute-solvent and solvent-solvent interactions evaluated through clusters isolated from solutions: Preferential solvation in water-alcohol mixtures

A. Wakisaka [a], S. Komatsu [b], Y. Usui [b]

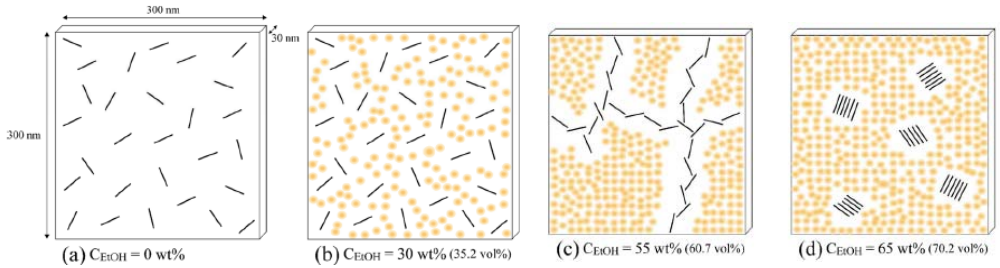
Supporting Evidence:
Clay Nanoparticles Induce Gelation in Alcohol-water Mixtures

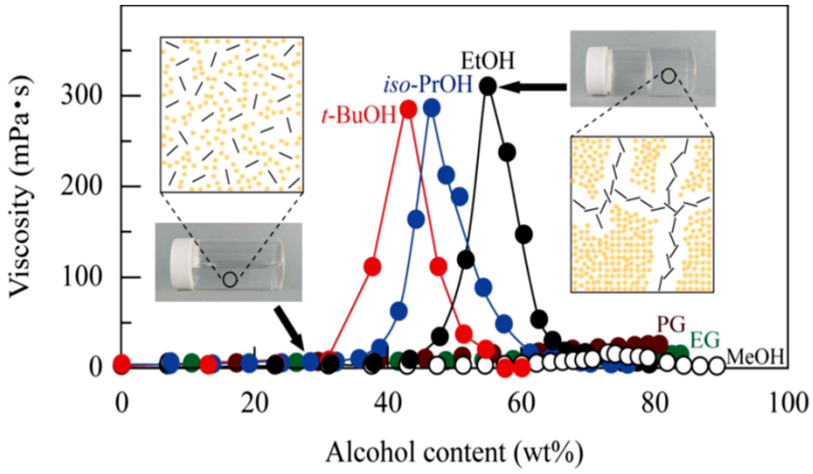
LANGMUIR Article
pubs.acs.org/Langmuir

Clay–Alcohol–Water Dispersions: Anomalous Viscosity Changes Due to Network Formation of Clay Nanosheets Induced by Alcohol Clustering

Yuji Kimura and Kazutoshi Haraguchi*

Department of Applied Molecular Chemistry, College of Industrial Technology, Nihon University, 1-2-1 Izumi-cho, Narashino, Chiba 275-8575, Japan





Kimura, Y. and Haraguchi, K., 2017. Clay–alcohol–water dispersions: anomalous viscosity changes due to network formation of clay nanosheets induced by alcohol clustering. Langmuir, 33(19), pp.4758-4768.

Impact of the Alcohol Type

- A lower alcohol concentration is required to form a gel with a more hydrophobic alcohol

Table: Octanol/Water partition coefficients for various alcohols and the respective concentrations required to form solid gels

Alcohol Type	Octanol/Water Partition Coefficient *	Alcohol Concentration
Methanol	-0.52	73%
Ethanol	-0.16	64%
Isopropanol	0.25	54%
Tert-Butanol	0.54	49%

** Serban Moldoveanu, Victor David, Modern Sample Preparation for Chromatography, Elsevier,2015, 131-189*

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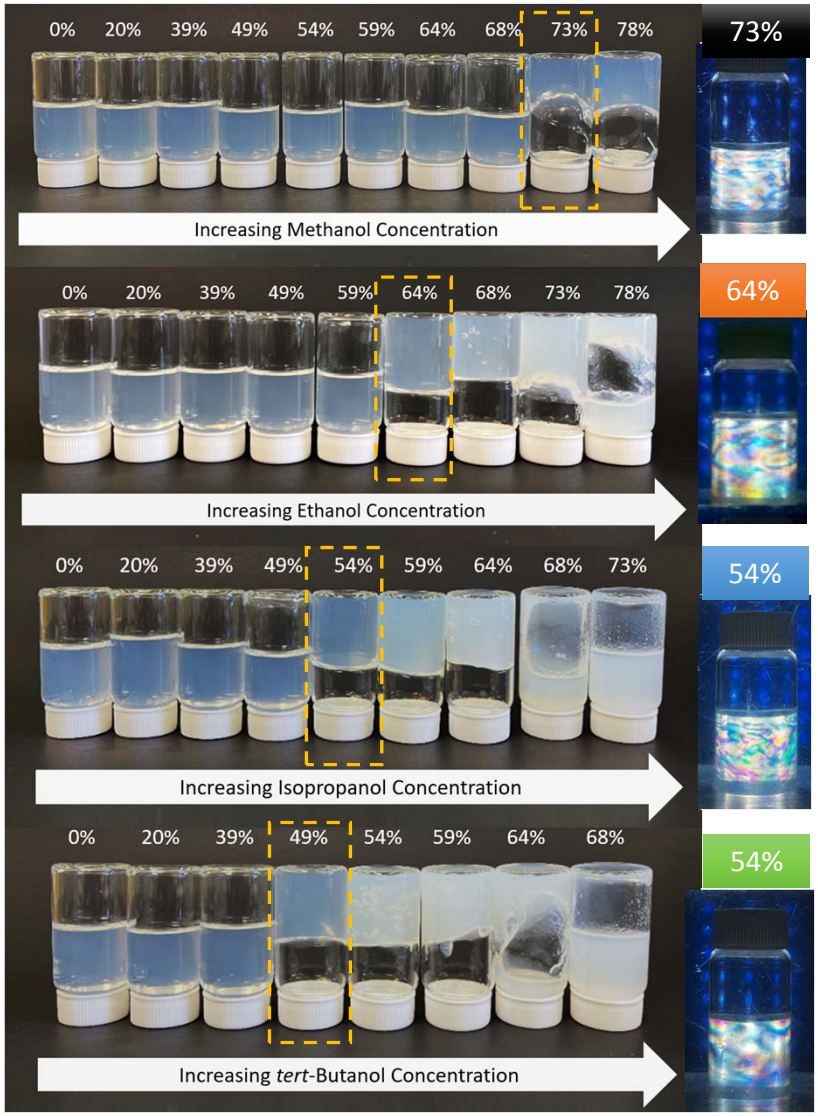
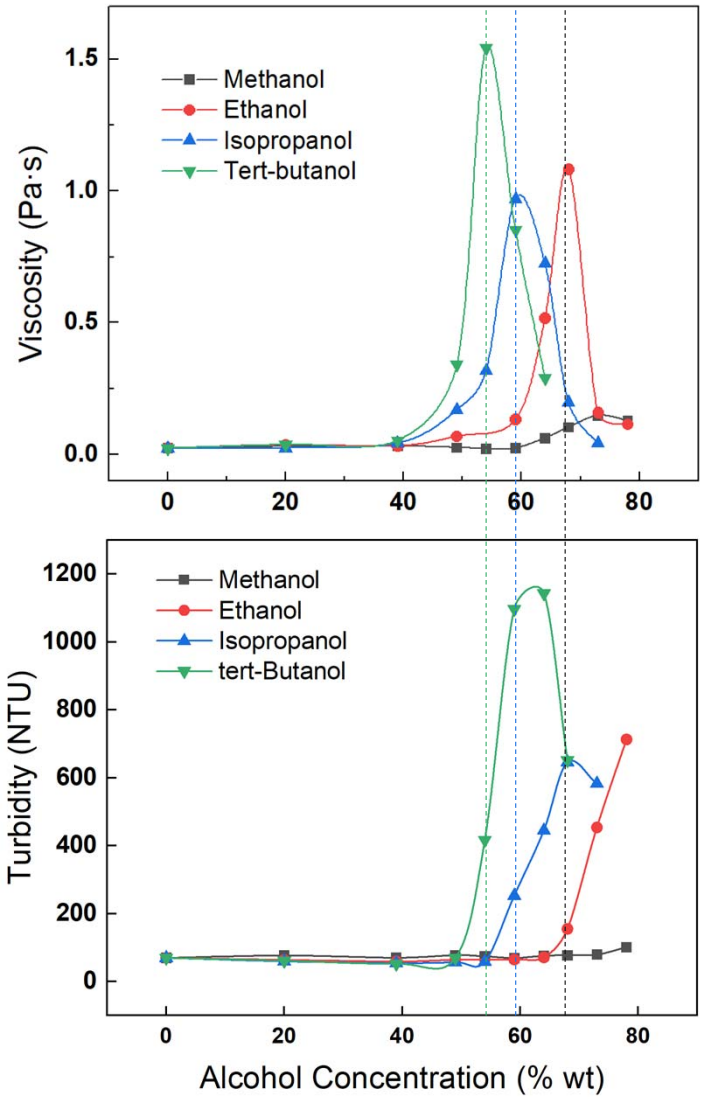


Impact of the Alcohol Type

- For all alcohol types at fixed 1.4%wt C_{CNC}
- A viscosity maximum is reached at a threshold alcohol concentration C_{max} , beyond which the viscosity decreases sharply
- Turbidity remains low until C_{max} , beyond which it increases sharply



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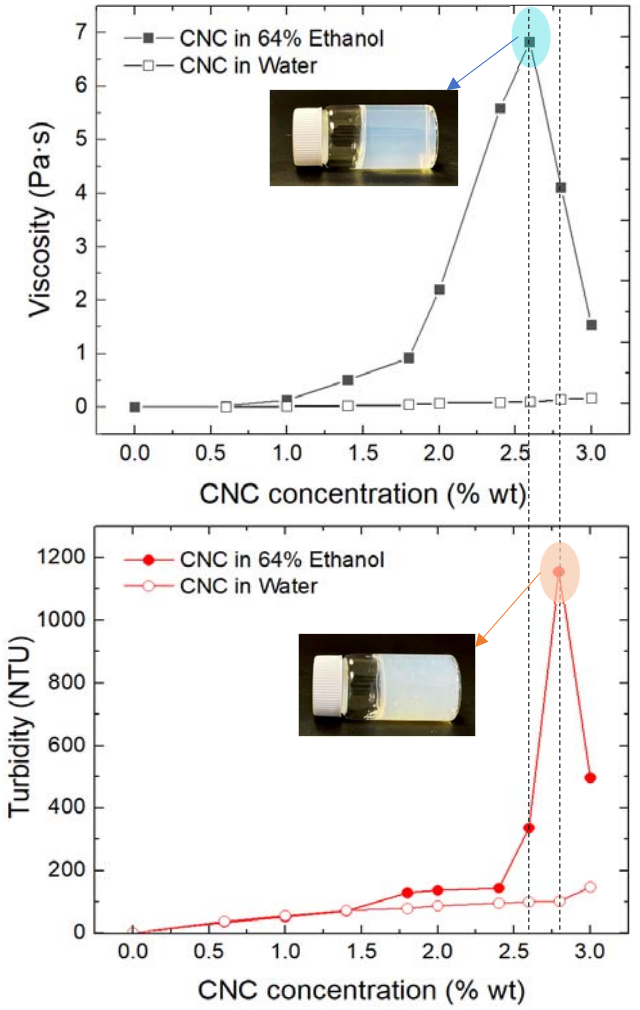
Impact of CNC Concentration

- Similar sharp increase in viscosity and turbidity was observed by increasing the CNC concentration at a fixed 64% $C_{Ethanol}$
- A maximum of viscosity and turbidity was observed at 2.6%wt and 2.8%wt CNC
- No significant change in viscosity (no gelation) and turbidity with increasing CNC concentration in the pure CNC-water system



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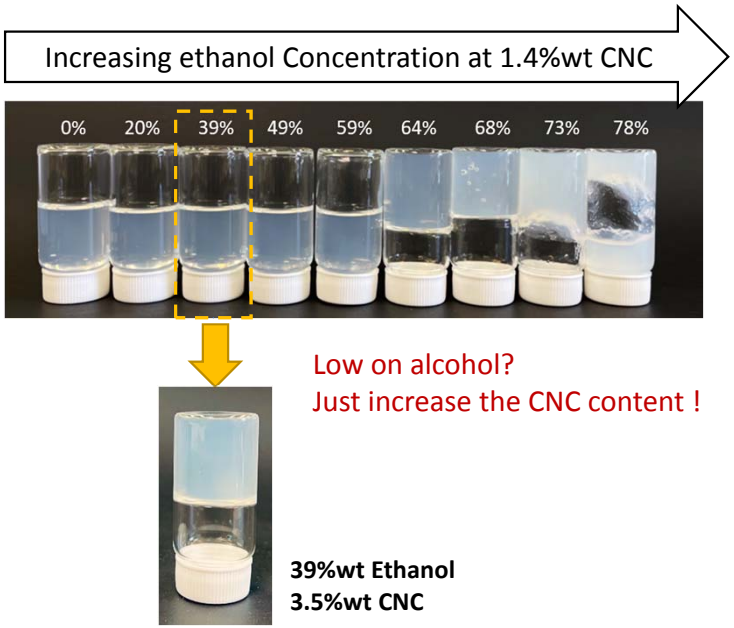
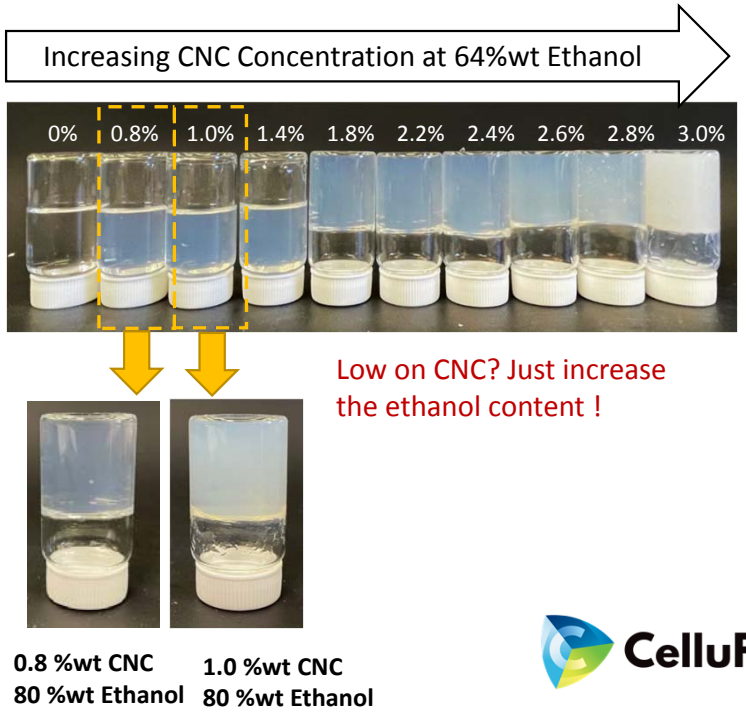
CNC-HAG: Formulation Tips

- Due to the water-depletion-induced-gelation mechanism, increasing either CNC concentration or alcohol concentration will facilitate gel formation.





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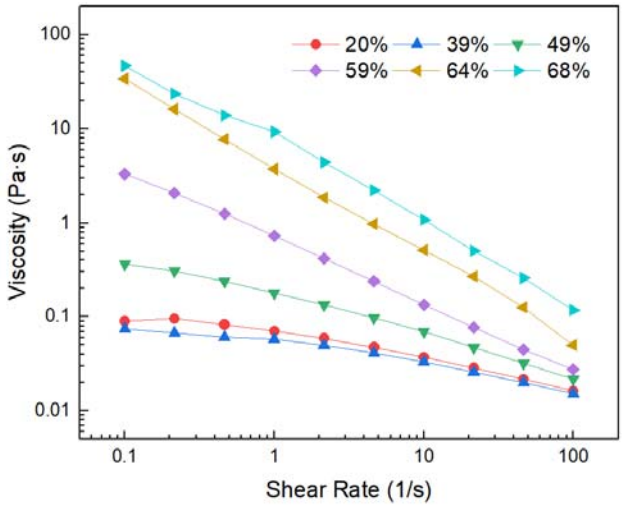
CNC-HAG: A Shear Thinning Gel

- Aqueous/alcohol dispersions of CNCs are shear-thinning.
- The thixotropic behavior is beneficial for the hand sanitizer application (*allows pumping from the bottle and spreading on the skin*)



✓ Easy to dispense
✓ Spreads smoothly

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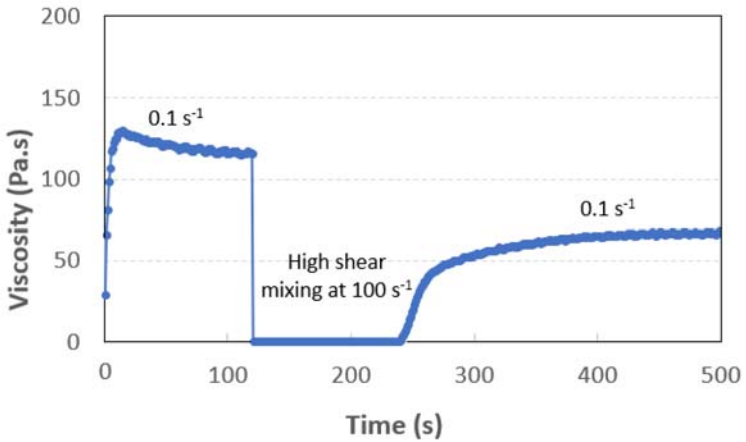
CNC-HAG: Gel Recovery

- The CNC-HAG gel shows a fast recovery after being high sheared
- Rapid recovery ensures that the hand sanitizer has a good retention on your skin once pumped and spread



Recovery curve for HAG containing 1.68%w/v CNC, 70% v/v Ethanol

✓ Has body
✓ Covers well

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Can CNC make a Good Gel Hand Sanitizer?

- ☑ Sanitizes
- ☑ Easy to dispense
- ☑ Has body
- ☑ Spreads smoothly
- ☑ Covers well
- ☑ Emolliates
- ☑ Cost effective
- ☑ Sustainable

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THANK YOU!