Nanostructure-Enhanced Phase Change Materials (NEPCM)

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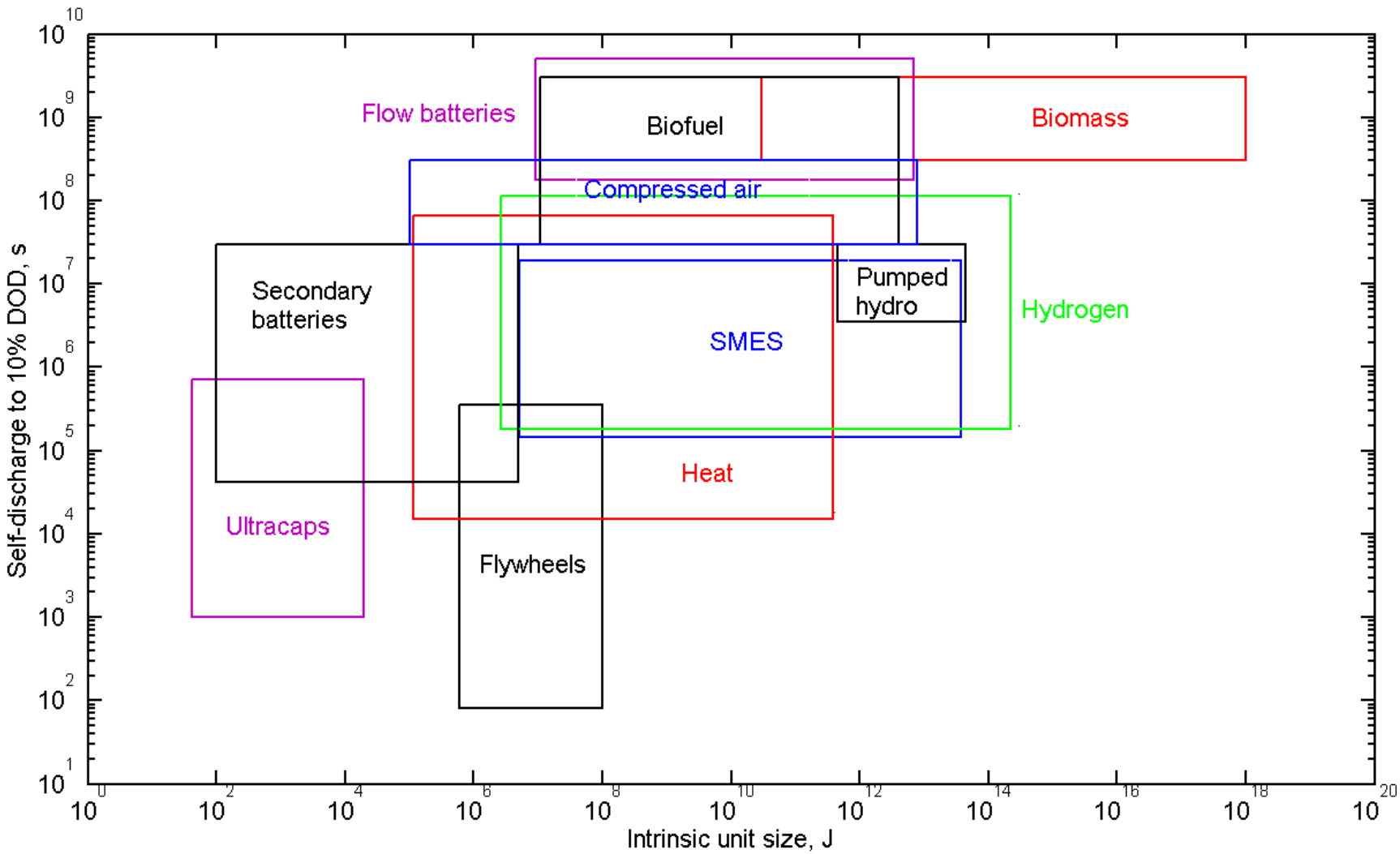
DoE EPSCoR Program Review 2009
Hosted by the
Brookhaven National Laboratory

July 20-23, 2009

Collaborators

Collaborators	
DoE National Laboratories	**ANL, ORNL, LBNL and INL**
Consultant	**Dr. Steve U. S. Choi (formerly with ANL, 1983-2006)**
Industries	**BASF, INTEL, Artic Silver, CTC and ICA**
Science Centers (SouthEast) and Pre-College Education (AL)	**McWane Science Center (Birmingham) Gulf Coast Exploreum Science Center (Mobile) Alabama Science in Motion (ASIM)**

Energy Storage Technologies



Source: R. Hammerschlag and C. P. Schaber, "Energy Storage Technologies," in Energy Conversion, Edited by D. Y. Goswami and F. Kreith, Chapter 15, CRC Press, pp. 15-1 to 15-22, 2008.

Rationale for Storage of Thermal Energy

Storage of Energy is required for managing any form of renewable sources of energy.

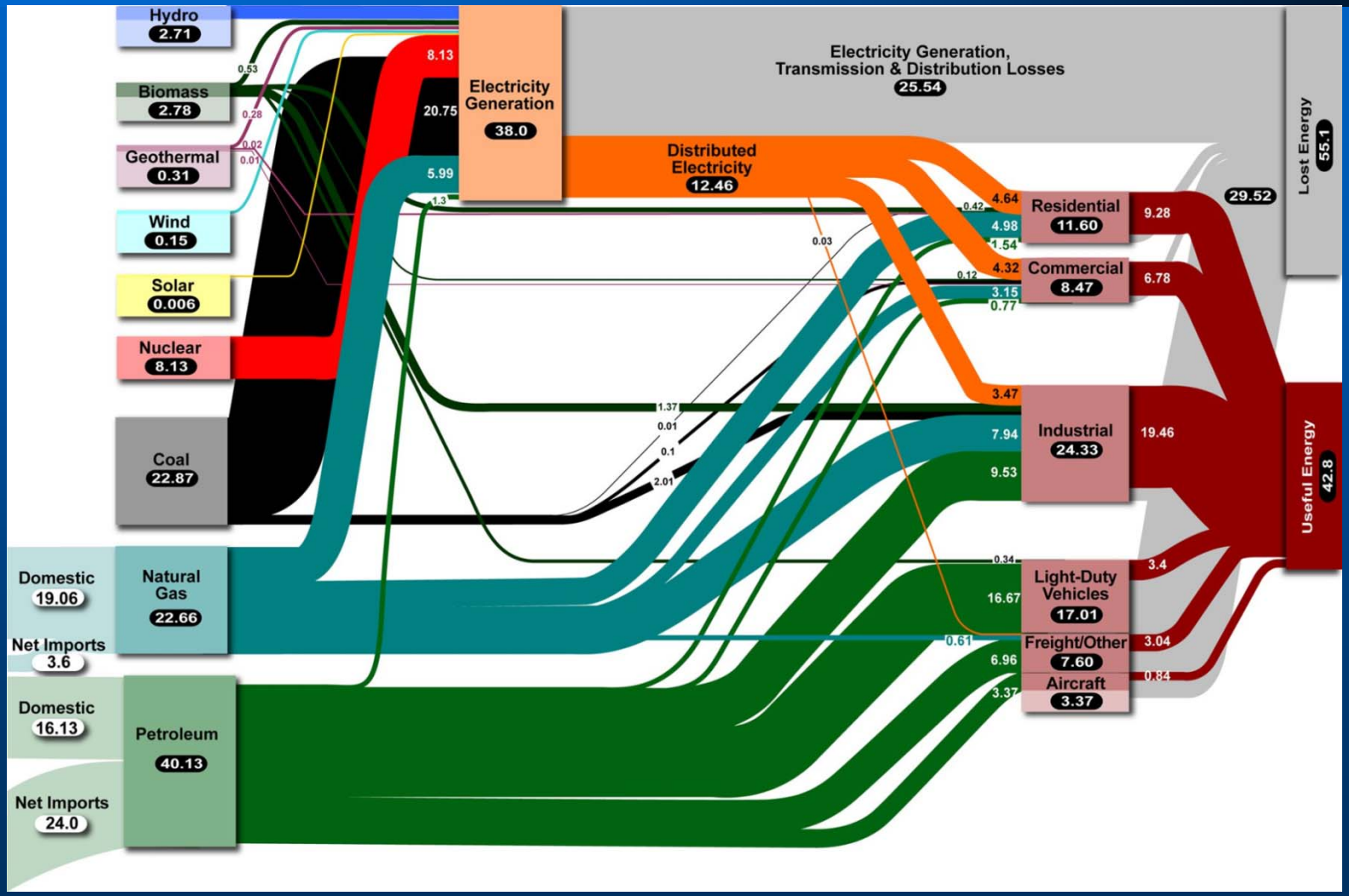
Thermal Energy is:

- Encountered in Nature (solar radiation, geothermal, stratified layers in oceans)
- Produced by all forms of energy conversion processes; widely labeled as “waste heat”

Storage of thermal energy is critical to:

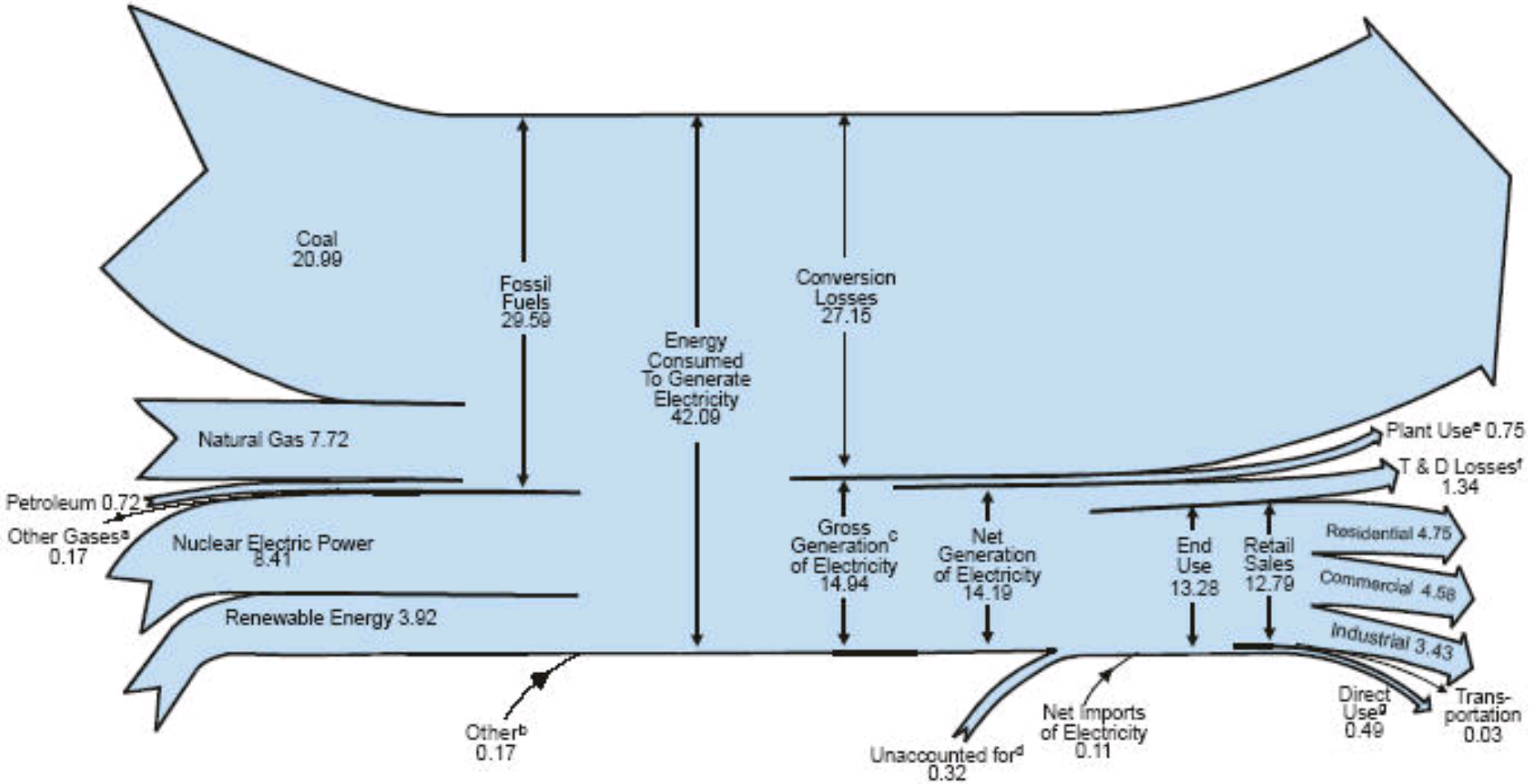
- Solar Thermal Power Plants
- Thermal Comfort (Residential/Commercial Sectors, Transportation, Textiles)
- Thermal Management of Electronics/Batteries

Primary Energy Sources and End Uses in the US (2002)



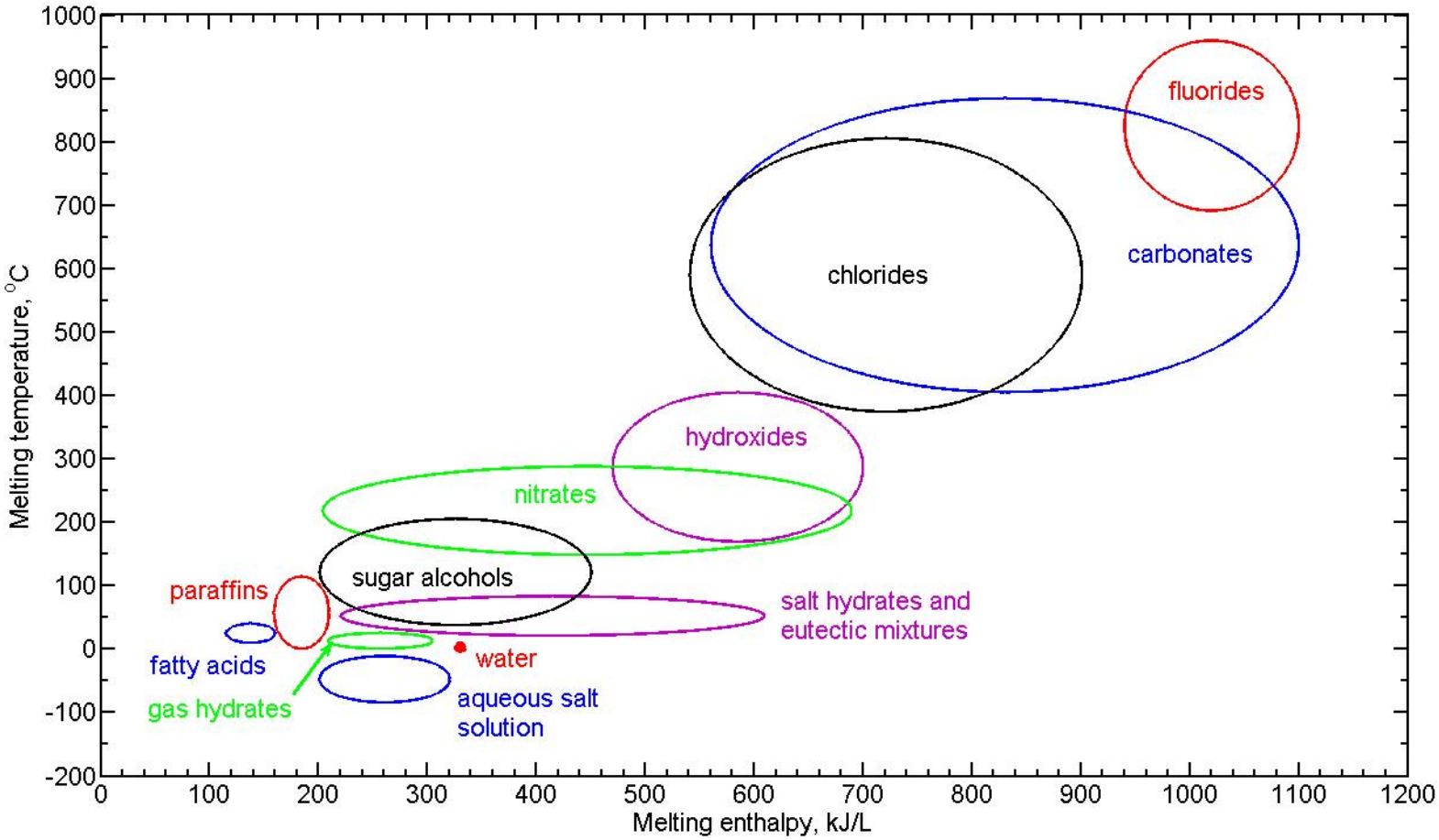
Source: https://eed.llnl.gov/flow/ {January 24, 2006}.

Electricity Flow, 2007 (Quadrillion (10^{15}) BTU)



Source: Annual Energy Review 2007, Report DoE/EIA-0384; http://www.eia.doe.gov/emeu/aer/diagram5.html

Thermal Energy Storage by Phase Change Materials (PCM)



Source: H. Mehling and L. F. Cabeza, "Phase Change Materials and Their Basic Properties," in Thermal Energy Storage for Sustainable Energy Consumption, Edited by H. A. Paksoy, Chapter 17, Springer, 2007.

Desirable Features of PCM

- High Latent Heat
- High Thermal Conductivity
- High Density
- High Specific Heat
- Low Volume Change
- Low Vapor Pressure

Enhancement of Thermal Conductivity of Paraffin Wax

- The thermal conductivity of typical paraffins is around 0.2 W/mK that is relatively low. (Water: 0.6, Aluminum: 235)

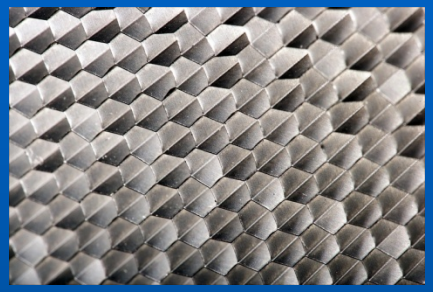
- Two pathways to enhance the effective *k*:

  - Introducing Fixed Structures, e.g., high thermal conductivity metal fins/fibers/foams, graphite

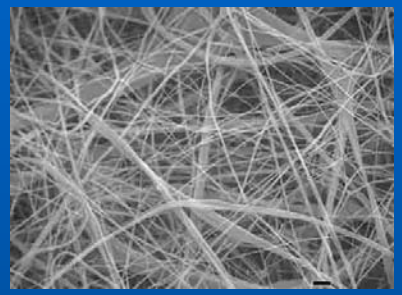
  - Suspending high thermal conductivity Particles (Nanoparticles).

Possible Routes to Enhance Thermal Conductivity of PCM

PCM (liquid) +

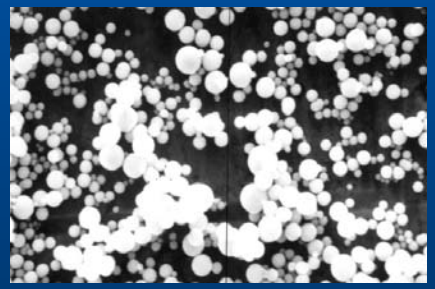


1 ~ 10 mm



Micron range

PCM/Metal composites

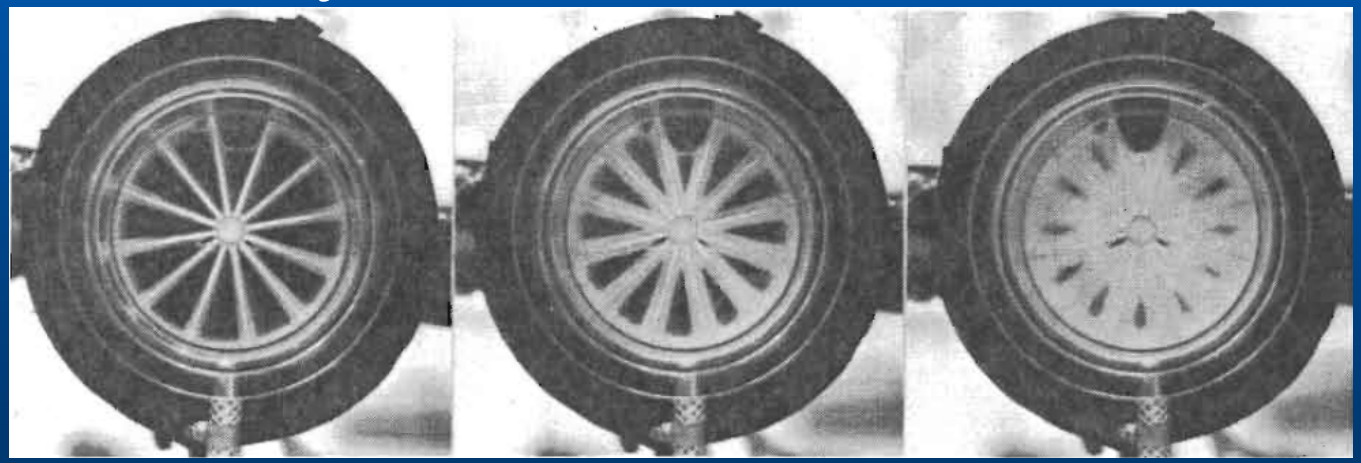


Particle-suspended PCM

Apparent Thermal Conductivity of PCM composites

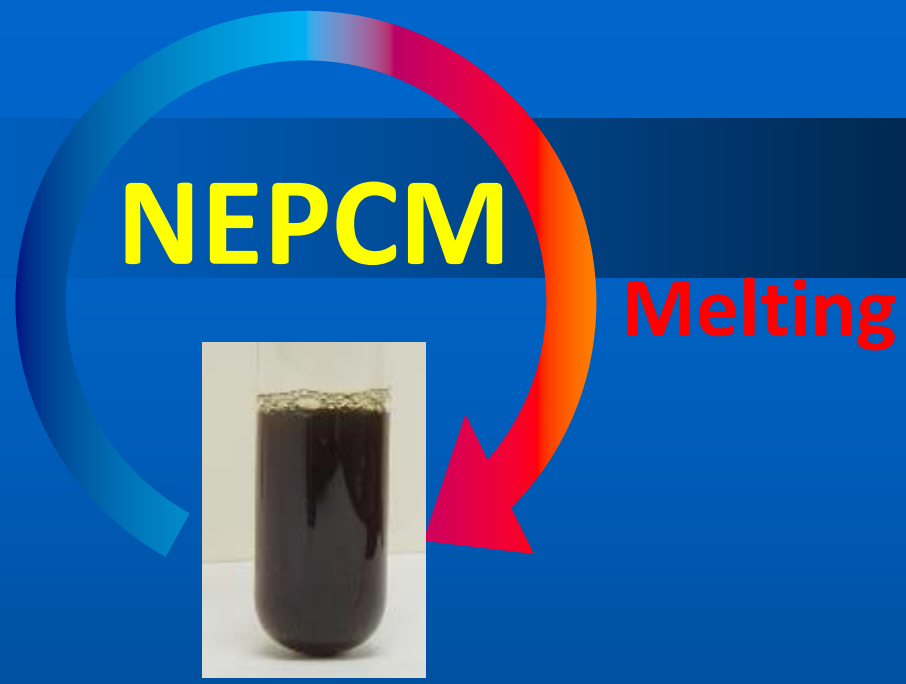
Introducing Fixed Structures

- Early work can be traced back to Bentilla *et al*. (1966) and Humphries and Griggs (1977) [both NASA reports.]
- Fillers: aluminum/copper fins, foams and honeycombs.



Transient freezing of the test model for solar storage with Eicosane (Abhat *et al*., 1981)

- A complete review of work on this topic is being prepared for publication [to be submitted to *Renewable and Sustainable Energy Reviews*.]



Advantages Compared to Graphite-Paraffin Composites

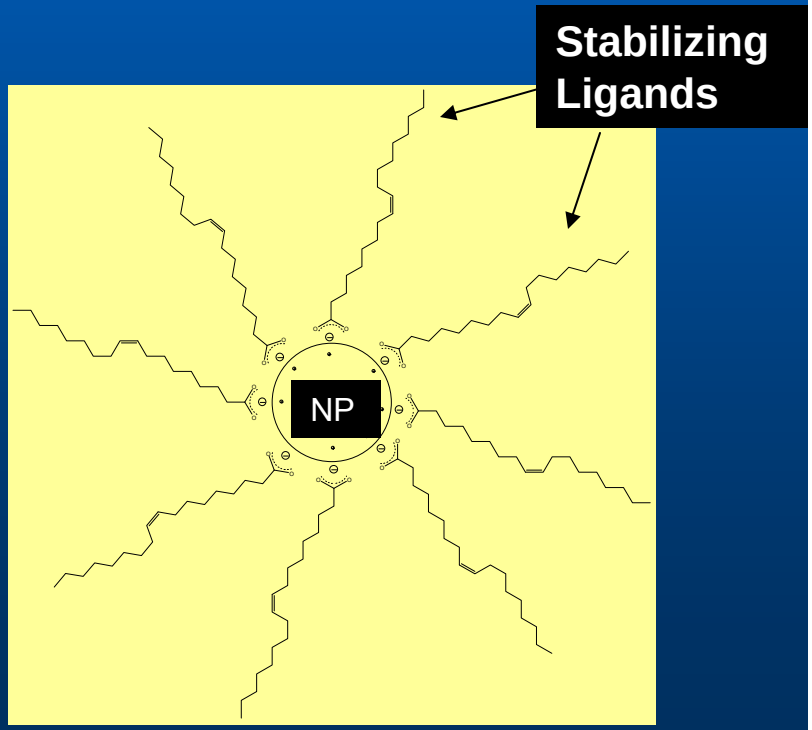
- Lighter weight,
- Higher latent heat,
- Availability of natural convection to enhance heat transfer upon melting,
- No “contact heat transfer” issues,
- Easy recycling.

Thrusts of the NEPCM Cluster

- Development, Characterization, Modeling & Testing
  AUBURN UNIVERSITY
- Nanoparticles Separation/Reclamation
- Utilization of NEPCM in High-Flux Electronics and Chip-Level Cooling
- Multi-Scale, Multi-Physics Non-Continuum Modeling
- Thermal Conductivity and Heat Dispersion Effect of NEPCM
- Nanoparticle-Enhanced Lubricating Properties of Paraffinic Oils

NEPCM Strategy

- Suspend ligand-stabilized NP's in a hydrocarbon base fluid
  - NP = CuO
  - Ligand = Sodium Oleate (SOA)
  - SOA has 2 regions:
    - Polar head interacts with NP
    - Non-polar tail interacts with the non-polar base fluid



NEPCM Challenges

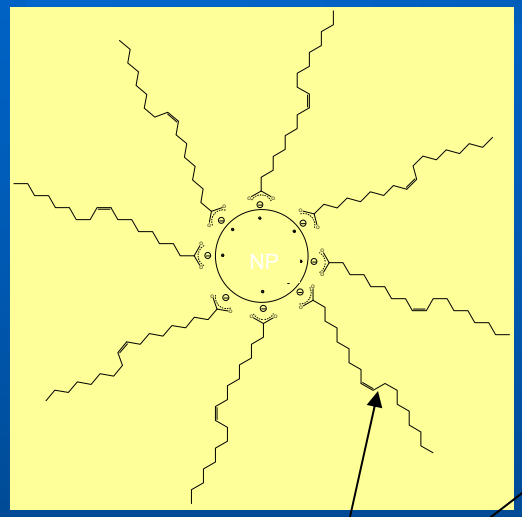
- Principal challenge is <u>colloidal stability</u>
  - Low concentration colloids can often be stabilized (10^{-3} % by mass)
  - High concentration colloids tend to precipitate (come out of solution)

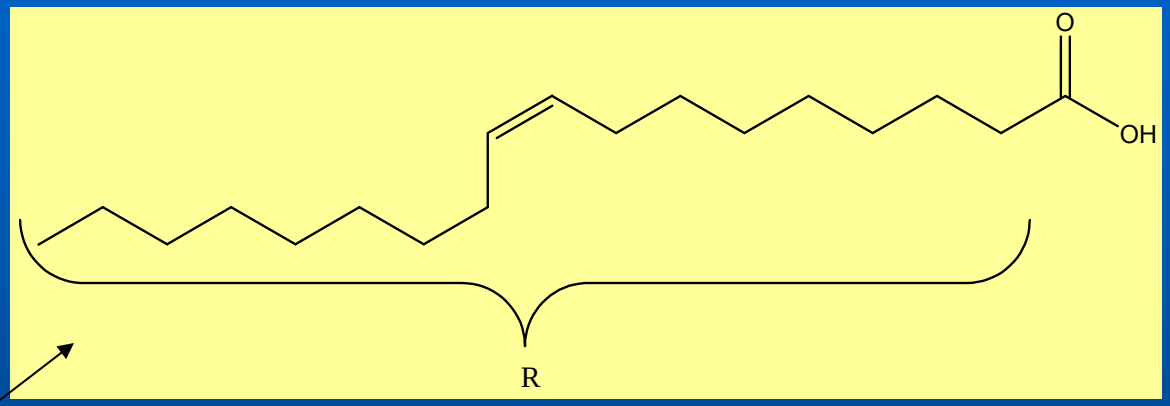
~0.04% (mass) CuO

2 Days →

$Cu(OH)_2$

CuO/SOA NP Preparation and Stabilization





Stabilizing Ligands

Particle

- $nCu(NO_3)_2 + 2nNaOH \rightarrow \mathbf{CuO}_n + 2nNaNO_3 + nH_2O$
- R—COOH + NaOH → R—COO-,Na+ + H_2O

  (Oleic Acid) (Sodium Oleate)

~1% CuO/SOA in Nujol Oil Stable at RT

- CuO/SOA 1 hour old

- CuO/SOA 8 months old

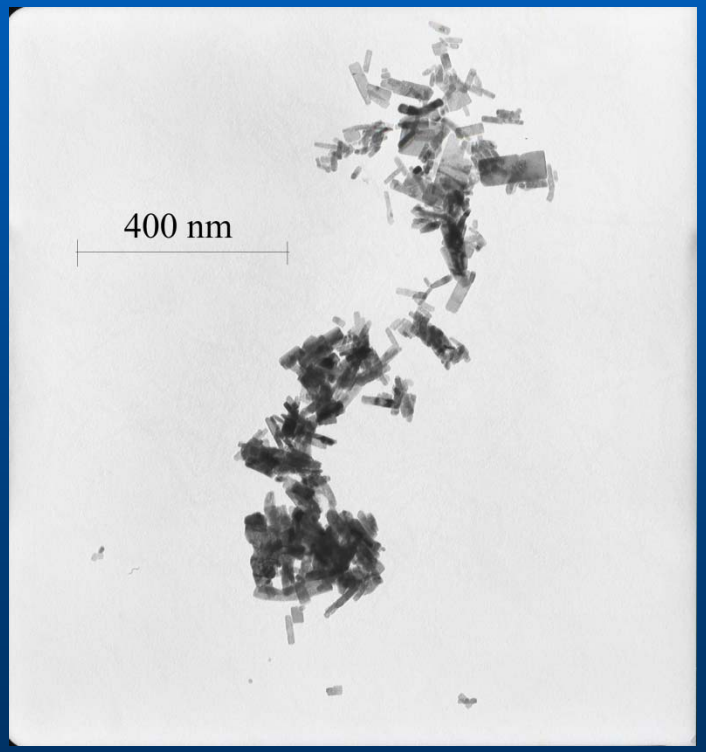
Current System—Freeze/Thaw Cycling

- CuO/SOA in Dodecane
- CuO/SOA in Nujol Oil

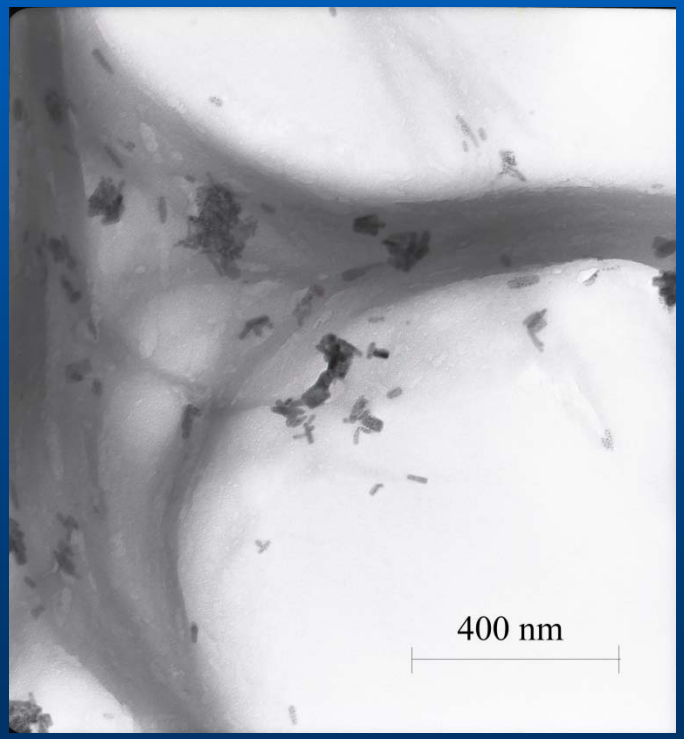
After 30 Cycles

CuO/SOA in Dodecane TEM

- Control

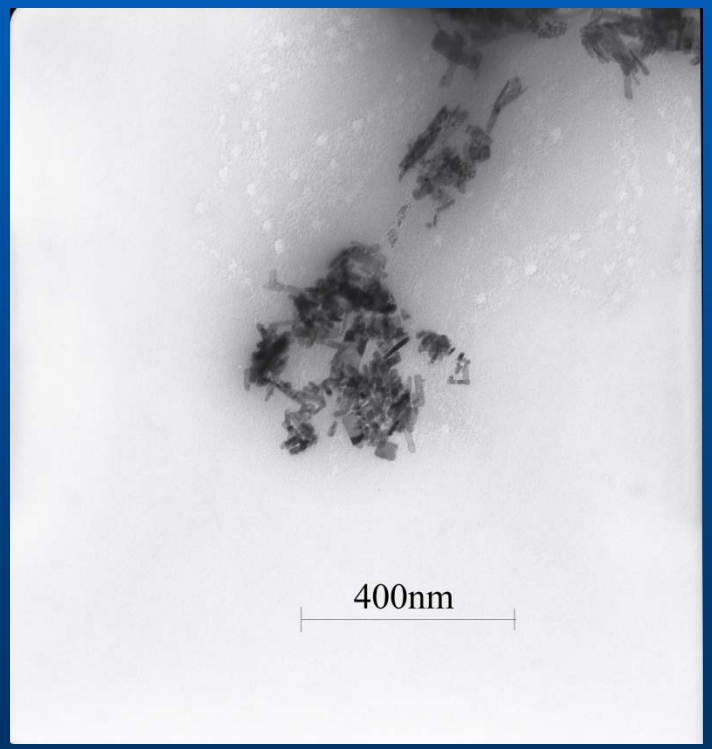


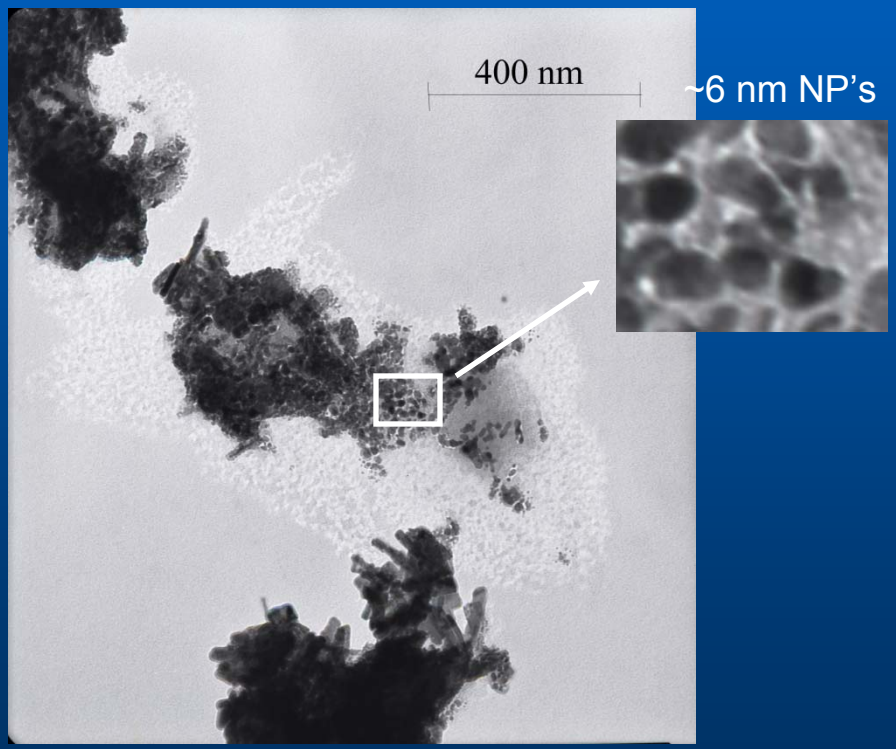
- After 30 Cycles



CuO/SOA in Nujol Oil

- Control
- After 30 Cycles

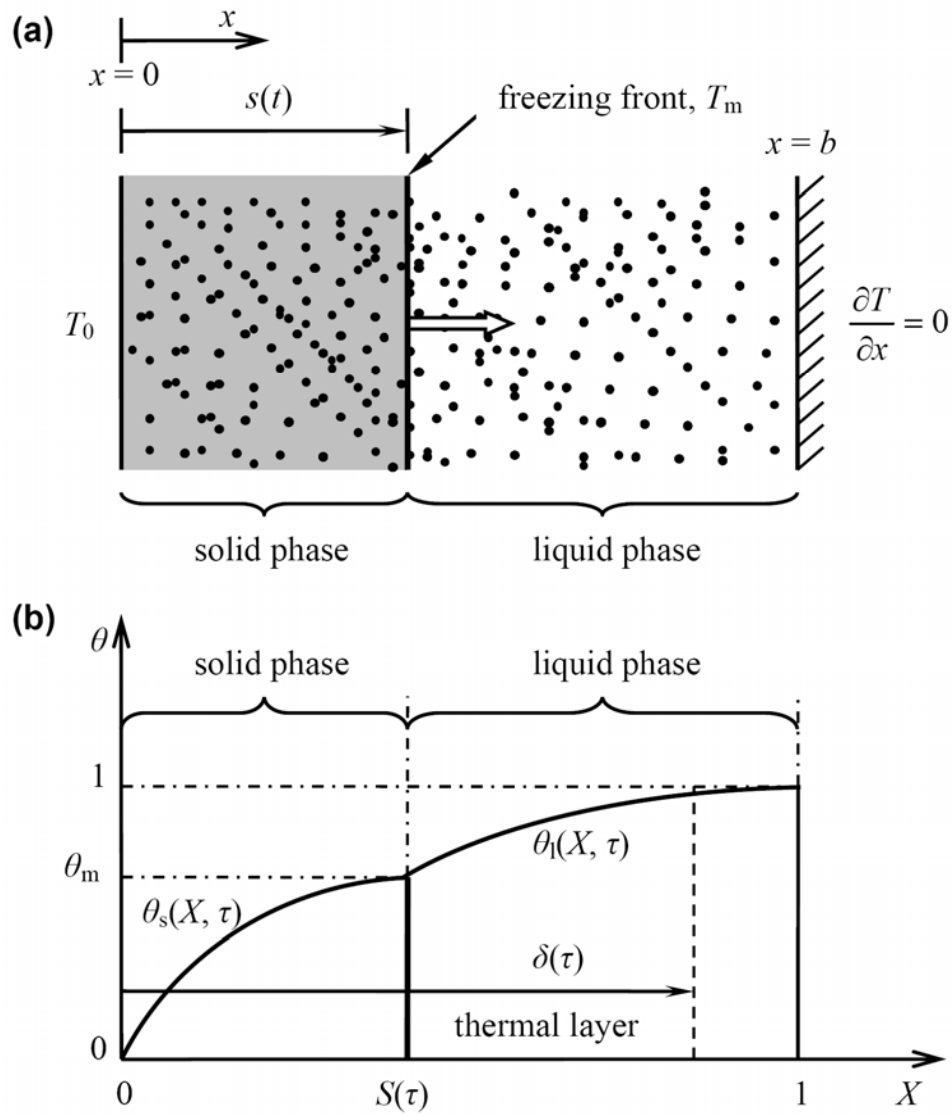




Characterization

- TEM
- Thermal Diffusivity
- Thermal Conductivity
- Specific Heat
- Melting Temperature
- Heat of Fusion
- Viscosity
- Laser Scattering and Small Angle X-ray Scattering (ANL)

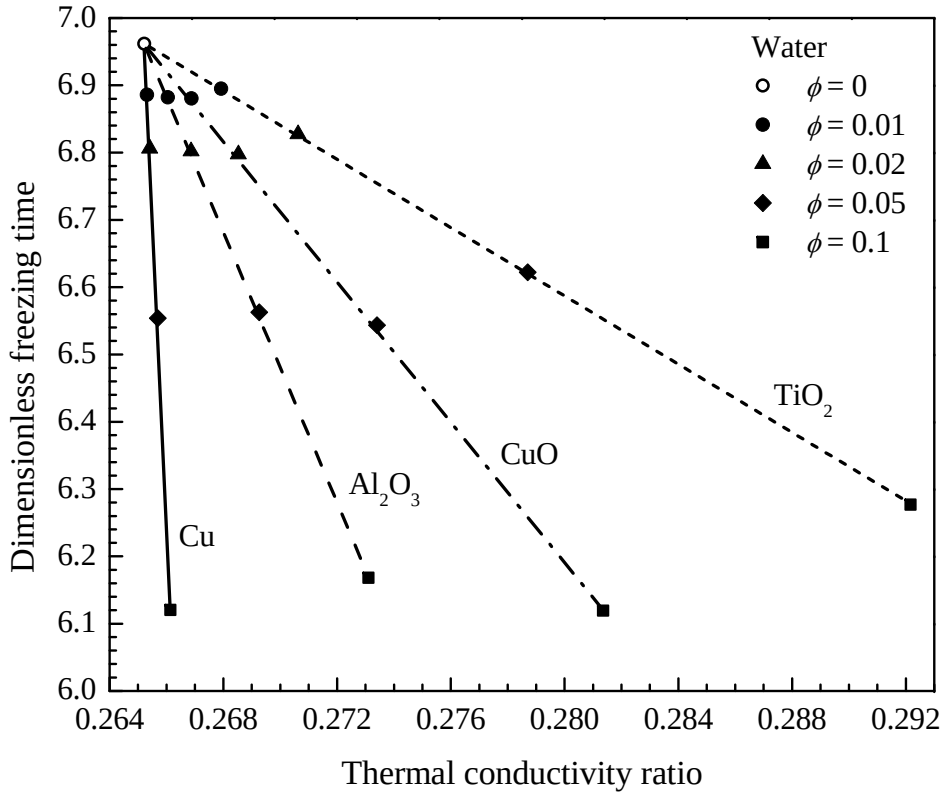
Schematic Diagram of the 1-D Stefan Model

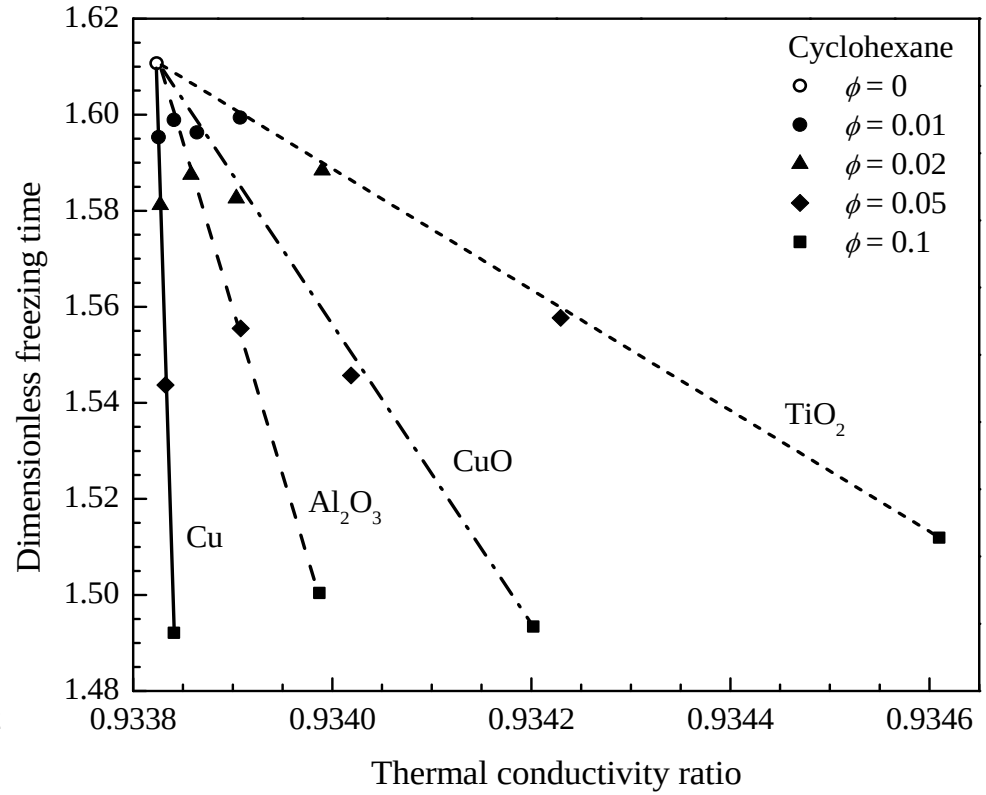


- Assume particle distribution remains uniform in both phases.

Schematic diagrams of:
(a) the physical model of the 1-D freezing of a slab and
(b) instantaneous dimensionless temperatures.

Results of the 1-D Stefan Model





(a) water (b) cyclohexane

Prediction of the effects of thermal conductivity ratio (liquid/solid) on the dimensionless freezing time of NEPCM thermal energy storage systems using the 1-D Stefan model.

Controlled Freezing Experiment

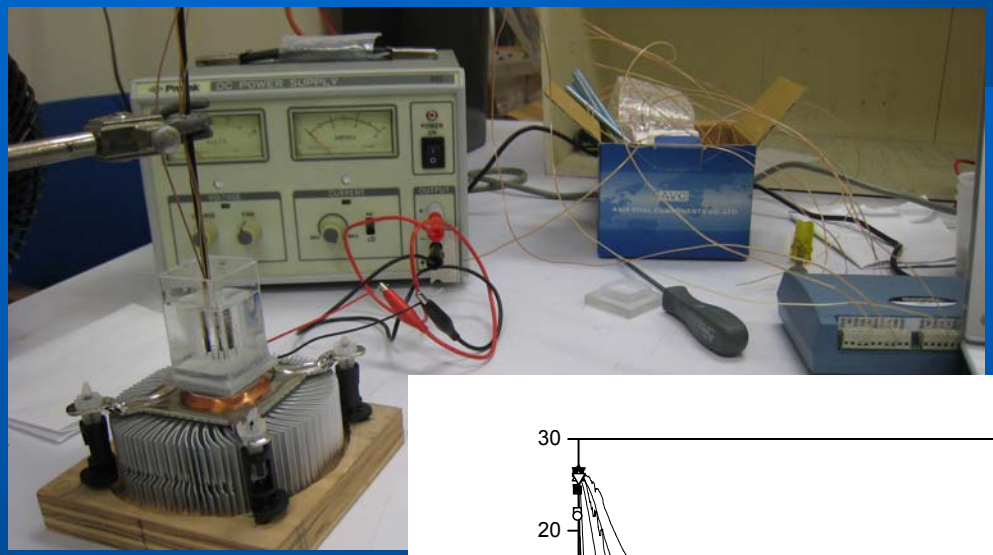
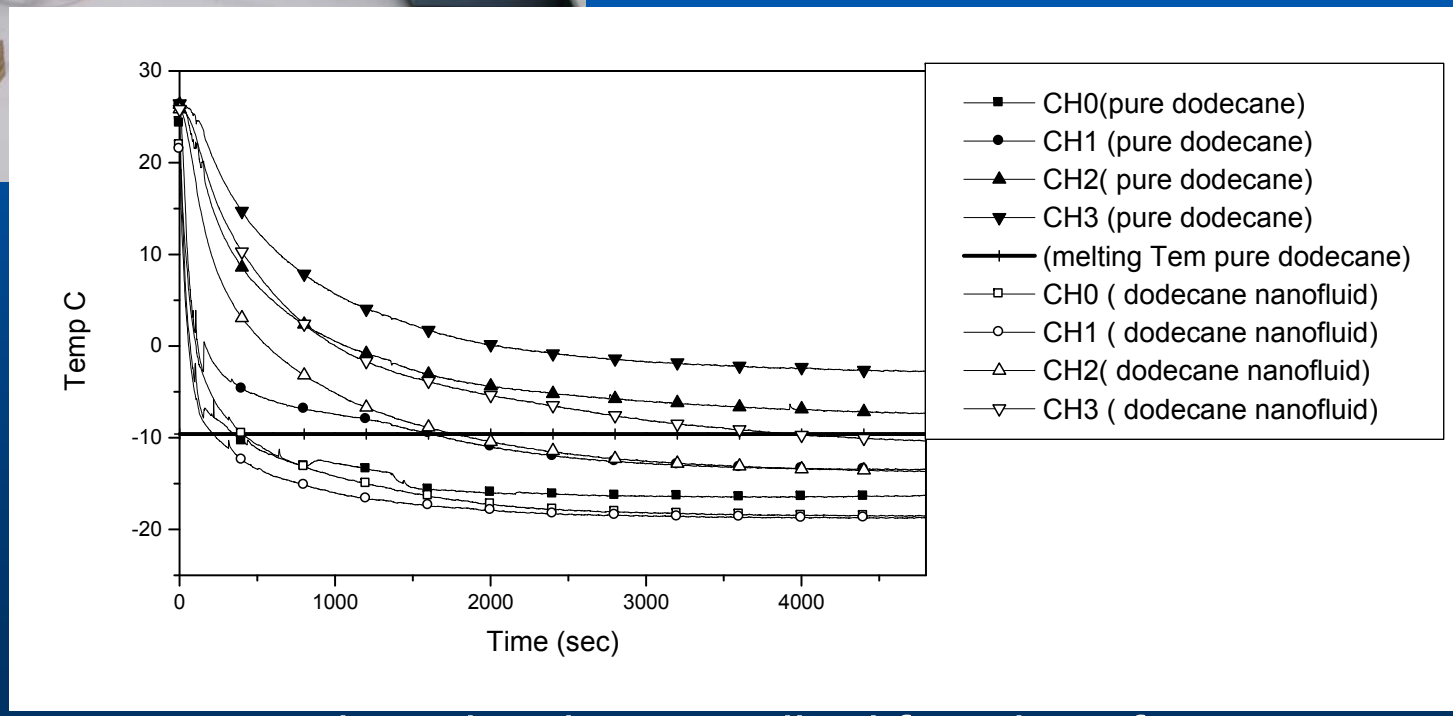


Photo of the set-up of the controlled phase change experiment

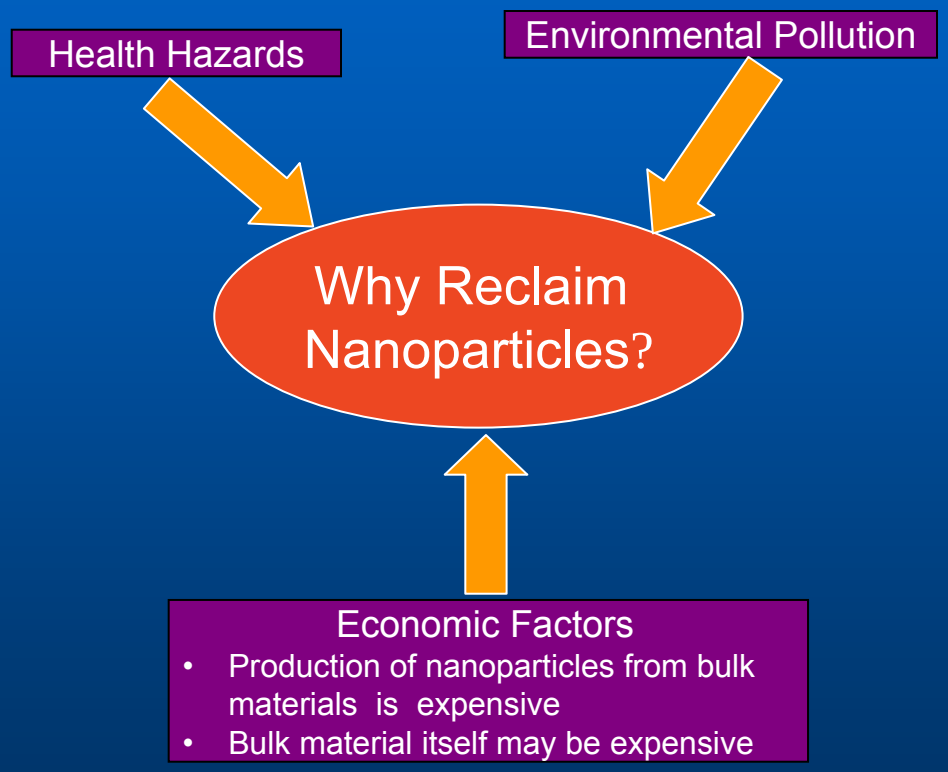


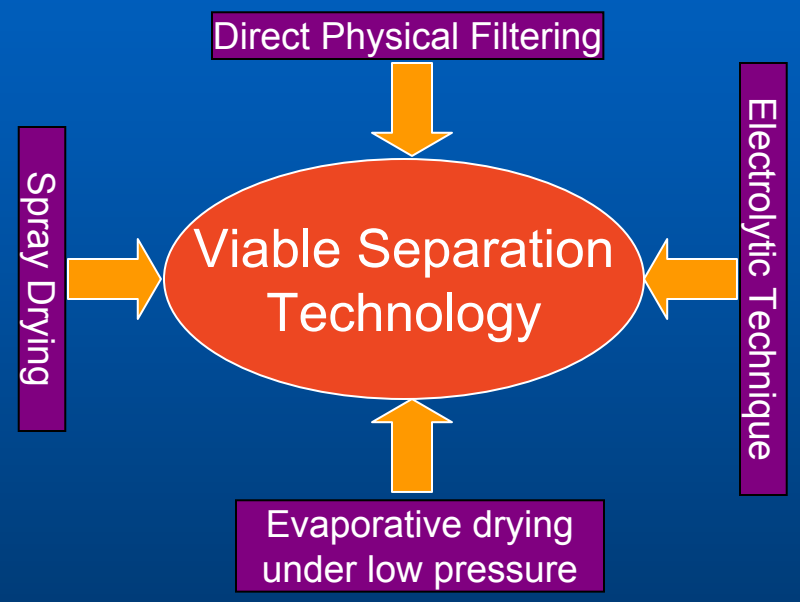
Experimental temperature data showing expedited freezing of a dodecane-CuO NEPCM in comparison to pure dodecane

Thrusts of the NEPCM Cluster

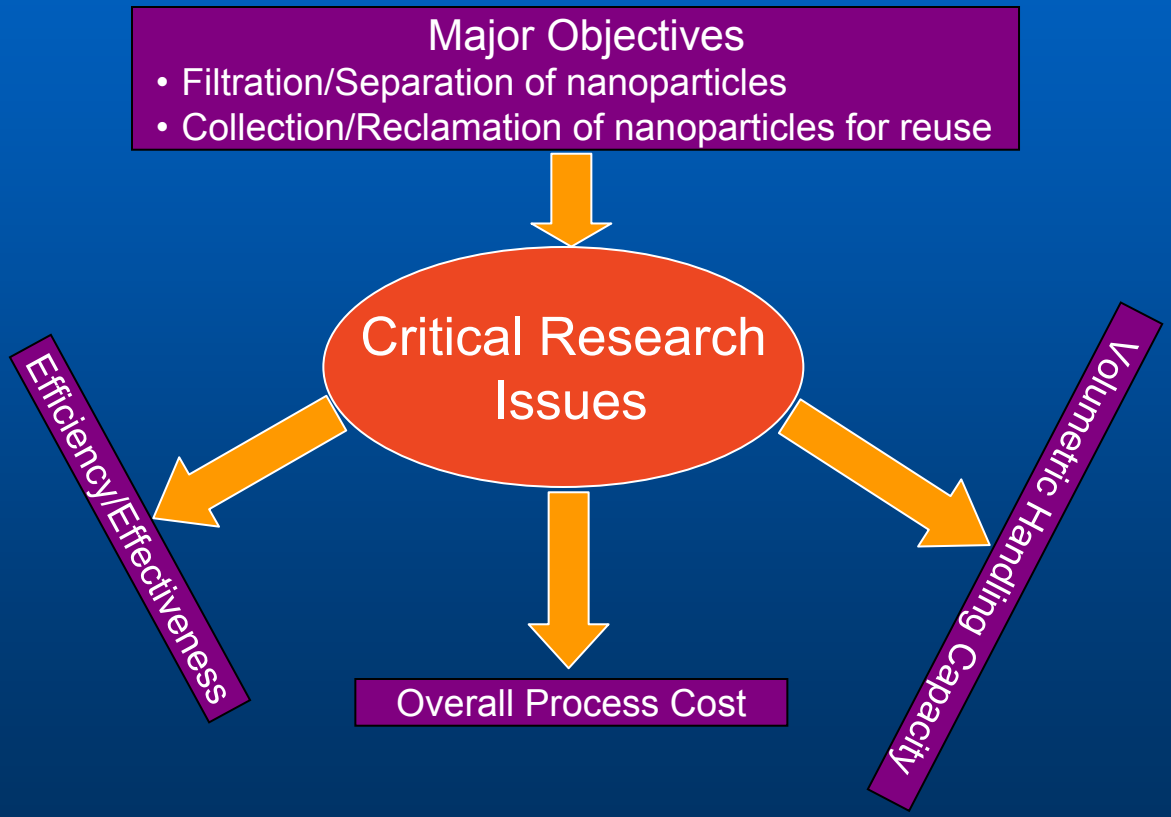
- Development, Characterization, Modeling & Testing
- Nanoparticles Separation/Reclamation
  The UNIVERSITY OF ALABAMA
- Utilization of NEPCM in High-Flux Electronics and Chip-Level Cooling
- Multi-Scale, Multi-Physics Non-Continuum Modeling
- Thermal Conductivity and Heat Dispersion Effect of NEPCM
- Nanoparticle-Enhanced Lubricating Properties of Paraffinic Oils

Nanoparticles Separation/Reclamation





Nanoparticles Separation/Reclamation



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  TUSKEGEE UNIVERSITY
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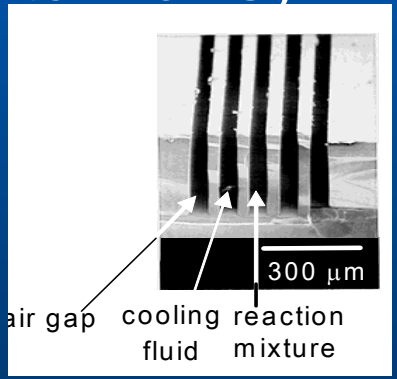
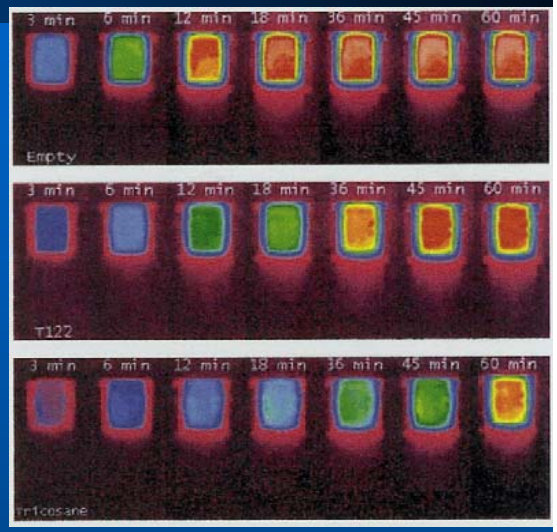
Utilization of NEPCM in High-Flux Electronics and Chip-Level Cooling

- Innovative Approaches to Thermal Management of Electronics
- Study NEPCM in relation to Improved Chip-Level Cooling (100 to -40 ^{o}C)

SEM Micrograph of DRIE MicroChannels Fabricated in a Silicon Wafer





Infrared Thermal Images of PCM-Cooled Electronics (bottom) compared to no PCM (top) and Thermasorb-122 (middle) (Hodes et al., 2002)

- Microfabrication in Consultation with INTEL
- Thermocouple/Heat Flux Sensors

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  AUBURN UNIVERSITY Montgomery
- Thermal Conductivity and Heat Dispersion Effect of NEPCM
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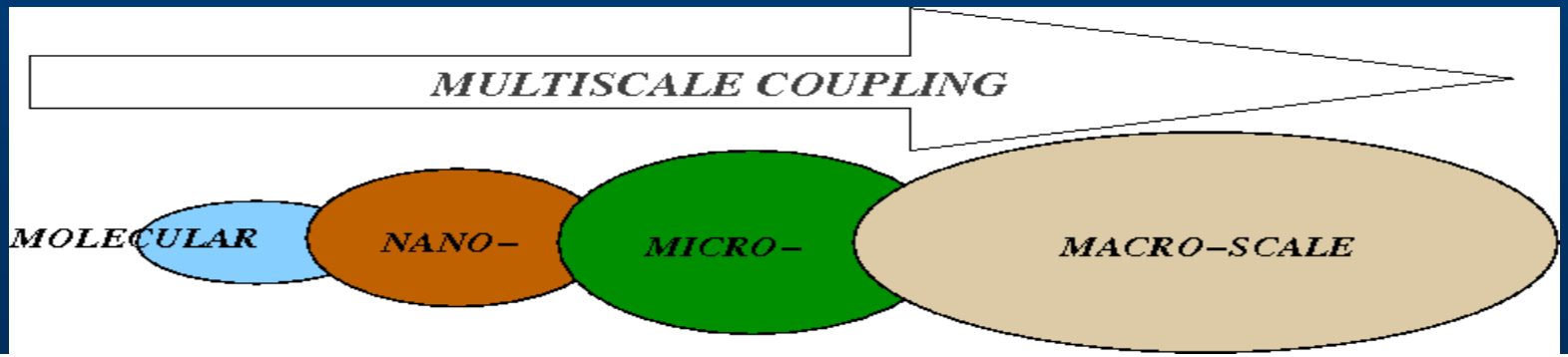
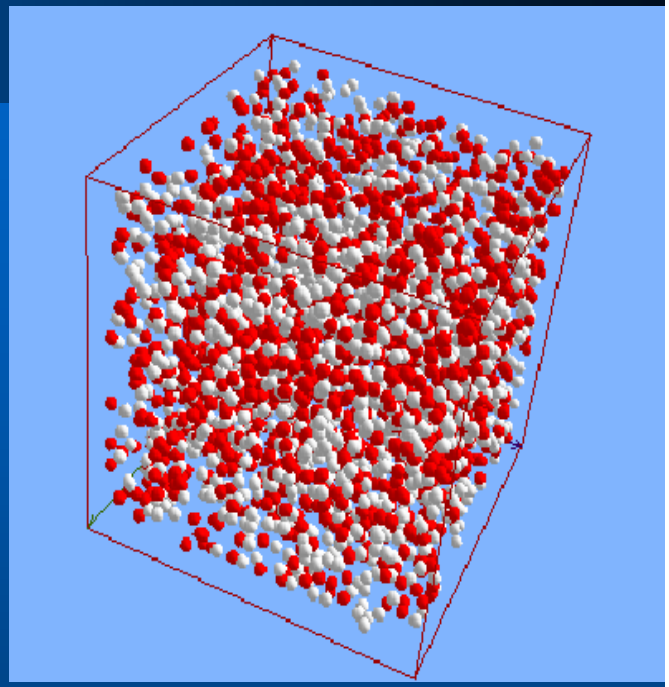
Multi-Scale, Multi-Physics Non-Continuum Modeling

- Methods:
  - Lattice Gas Automata (LGA)
  - Molecular Dynamics (MD)
  - Lattice Boltzmann (LB)
- Multi-Physics Analysis:
  - Heat Transfer + Fluid Dynamics + Thermodynamics
- Computer Implementation:
  - Parallel Codes (MPI/OpenMP)
  - Distributed (Grid Enabled) codes
  - Visualization



Multi-Scale, Multi-Physics Non-Continuum Modeling



- Thermal Properties to be predicted
  - Thermal Conductivity
  - Specific Heat Capacity
  - Thermal Diffusivity
  - Specific Latent Heat
    → Melting/Solidification Temperatures
- Other Properties
  - Viscosity
  - Nano-particle distribution (including temporal evolution)
    → Nano-particle Aggregation and Sedimentation
- Parameters
  - Pressure, Temperature, Flow, Particle Concentration

Major Thrusts of the NEPCM Cluster

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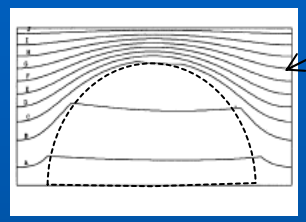
  UNIVERSITY OF SOUTH ALABAMA
- Nanoparticle-Enhanced Lubricating Properties of Paraffinic Oils

Thermal Conductivity and Heat Dispersion Effect of NEPCM

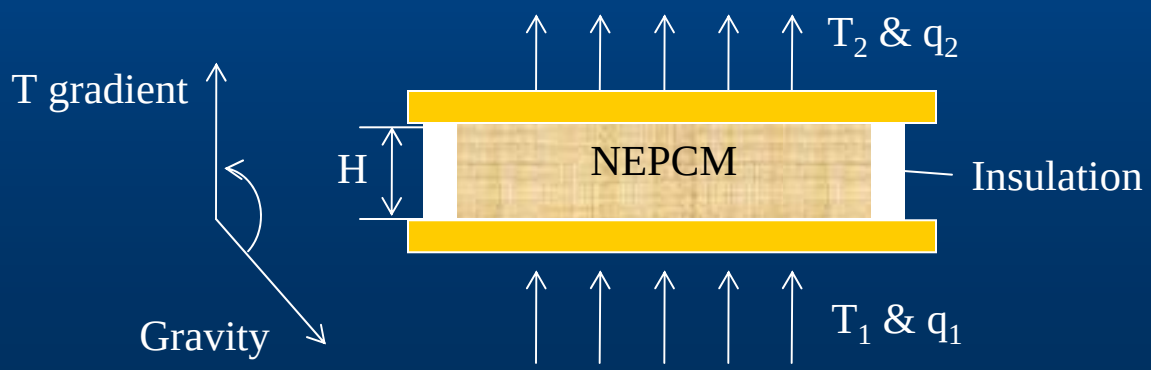
- Thermal conductivity enhancement of solid-state NEPCM

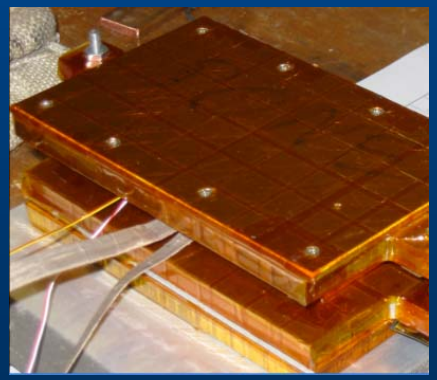
Average Temperature Gradient in NEPCM



Compression of Local Temperature Contours Due to the Highly Conductive Nanoparticle

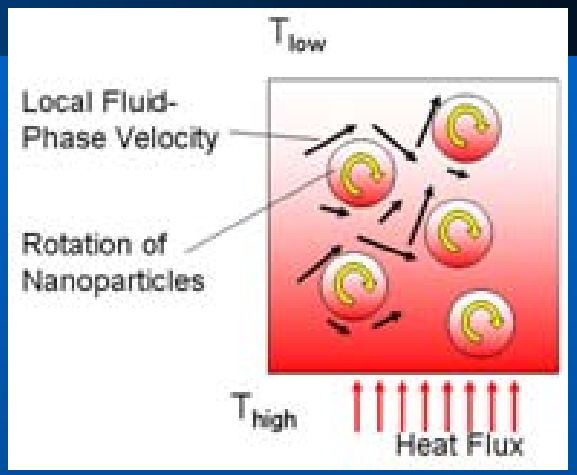
- Heat transfer enhancement due to natural convection of liquid-state NEPCM.
- Measurement Setup

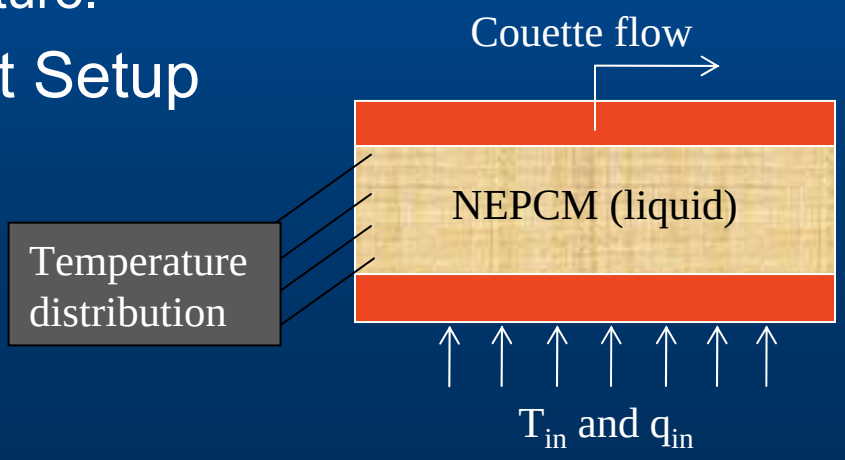




Thermal Conductivity and Heat Dispersion Effect of NEPCM

- Heat Dispersion in Flow of NEPCM
  - Enhanced macroscopic conduction due to non-uniform local liquid and nanoparticle motion/rotation.
  - High heat capacity of the nanoparticle
  - High latent heat of the phase-change matrix
  - Possible high heat transfer rate achieved with a small temperature gradient especially near the phase-change temperature.
- Heat Dispersion Measurement Setup





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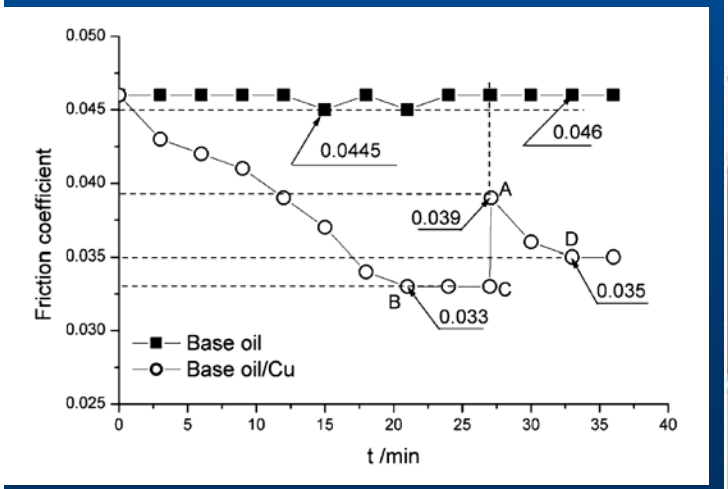
AUBURN UNIVERSITY

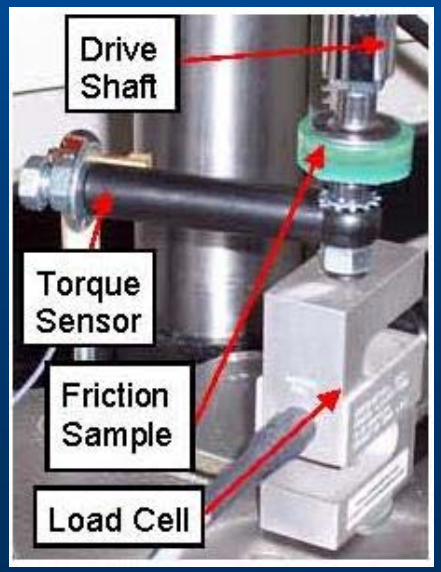
Motivation for Nanofluid Lubrication

- Reducing engine friction will improve fuel economy.
- 20-30% of the energy produced by a modern combustion engine is lost to friction.
- The DOE finds that merely a 5% reduction of engine energy losses would cut the consumption of oil by approximately 100 million barrels.
- This approach could allow for improved friction in not only new vehicles but vehicles currently on the road.
- **Current study will research nanoparticle usage in careful comparison to existing lubricating oil formulations.**



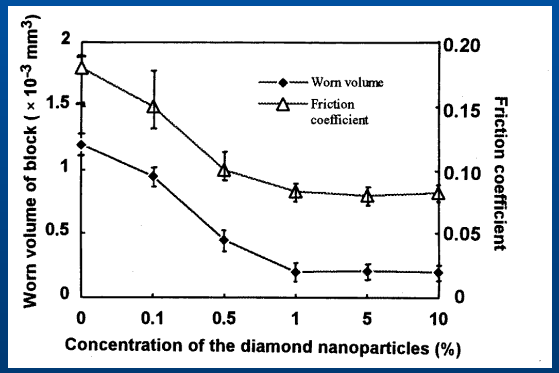
Liu et al. (2004)

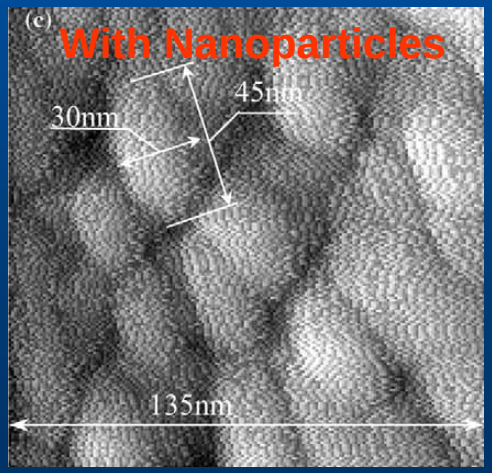
Auburn University Test Facilities

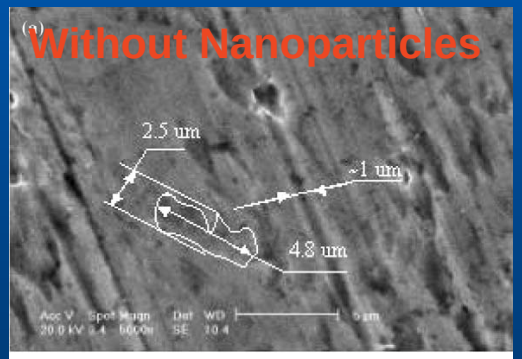


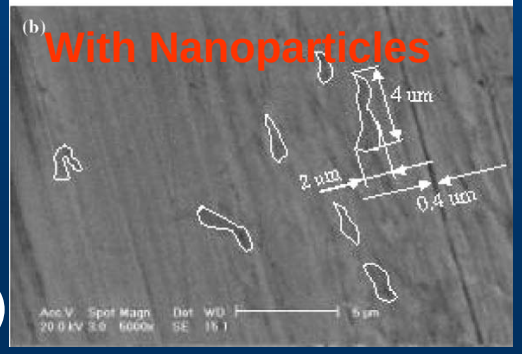
Nanoparticle Effects on Lubrication

- Nanoparticle lubrication enhancement mechanisms:
  - the particles may affect viscosity (Wu et al., 2007)
  - the particles affect the thermal properties and thermal stability (Hwang et al., 2006)
  - the particles could roll between the surfaces and act as “nano ball bearings” (Wu et al., 2007, Tao, Jiazheng, Kang, 1996) – Friction Reduction
  - the particles could mend worn surfaces by adhering to them (Liu et al., 2004, Wu et al., 2007)









Tao, Jiazheng, Kang (1996) and Liu et al. (2004)