10. 학사논문 지도교수: 여 재 익

10-1. [수치해석|sim.] Numerical analysis of the swirling flame in the gas turbine combustor

10-2. [수치해석|sim.] Multi-phase simulation based on DSC experiment

10-3. [수치해석|sim.] Numerical analysis of hypersonic combustion of solid fuel via scramjet combustor

10-3. [수치해석|sim.] Numerical analysis of metalized solid propellants on the meso-scale

10-4. [수치해석|sim.] Modeling of a long-range high-power laser-artillery shell interaction about fine dust and virus combined with deep learning

10-5. [수치해석|sim.] Numerical Modeling Physical Mechanism of ECSP Combustion

10-6. [실험|expt.] Dielectric breakdown-induced shockwave and its biomedical application

10-7. [실험|expt.] Experimental analysis of combustion behavior of electrically controlled solid propellants

10-8. [실험|expt.] Experimentally understanding the enigmatic combustion of electrically controlled solid propellants

10-9. [실험|expt.] Developing a prototype of FEEP Thruster for Nano-Satellite

10-10. [실험|expt.] Aging analysis for the energetic materials comprising of metal fuels

10-11. [실험|expt.] Prediction of thermal runaway characteristics by thermal analysis to secure the battery safety

10-12.[실험|expt.] Characterization of thermal runaway in ultrahigh-nickel lithium-ion battery from experiments and modelling

10-13. [실험|expt.] Experimental investigation on Taylor cone formation using different emitters for development of FEEP thruster

10-14.[실험|expt.] Comprehensive Study of the Thermal Runaway Characteristics of High-Energy Lithium-ion Batteries using Differential Scanning Calorimetry (DSC)

10-15. [실험|expt.] Thermochemical analysis of magnesium and magnesium-based mixture

10-1. [수치해석|sim.] Numerical analysis of the swirling flame in the gas turbine combustor (남재현, Jaehyun Nam)

- Swirling flame in the gas turbine combustor
  - Highly turbulent and complex flow structure
  - Used for the stabilization of flame
  - Possibly trigger combustion instabilities

- Simulation of the swirling flame in the gas turbine combustor requires
  - Large-eddy simulation (LES) turbulence eddy-viscosity model
  - Finite rate chemistry or flamelet reaction model
  - Three-dimensional modeling based on unstructured mesh
  - Parallel computing

- Investigation of the thermochemical process from simulation
  - Identify the qualitative and quantitative details of swirling flame
  - Parameterize the mixing and reacting process
  - Clarify the cause of the combustion instability
  - Investigate the effects of the numerical method

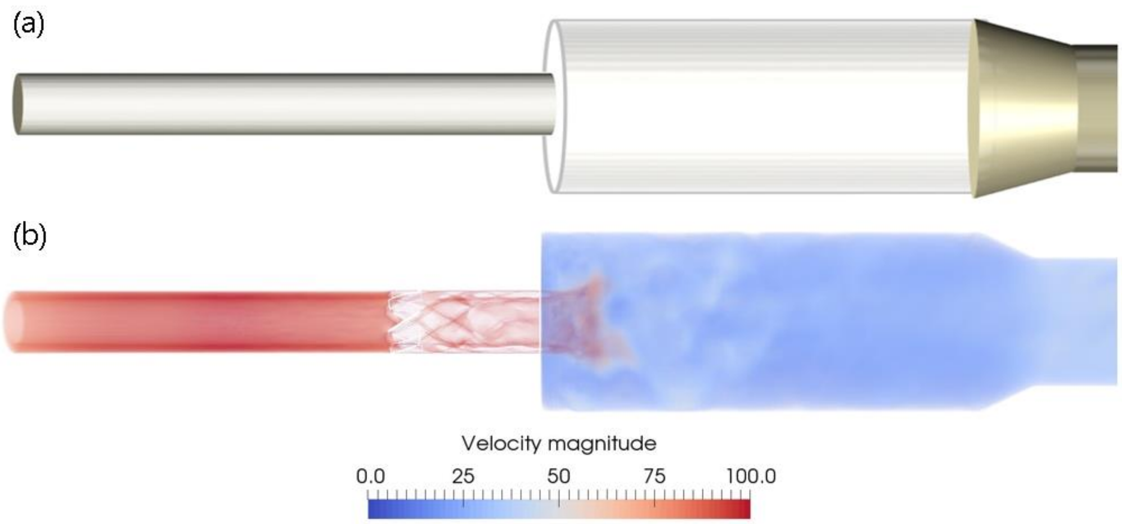


Fig. (a) Schematic of the gas turbine combustor and feedline and (b) LES result of the flow field in the combustor

담당조교 : 남재현 (wogus1336@snu.ac.kr)

10-2. [수치해석|sim.] Multi-phase simulation based on DSC experiment (남재현, Jaehyun Nam)

- representation of the chemical reaction velocity equation
  - For accurate computational simulation of high-energy materials composed of solid or liquid state
  - using the reaction kinetics which can be obtained by experimental data from differential scanning calorimetry (DSC)
  - chemical species variable calculated in the calculation code

- Identifying the characteristics of heat storage material systems based on DSC experiments
  - high computational efficiency of one step chemical reaction
  - very specific velocity expression variable that varies from mass fraction to fraction

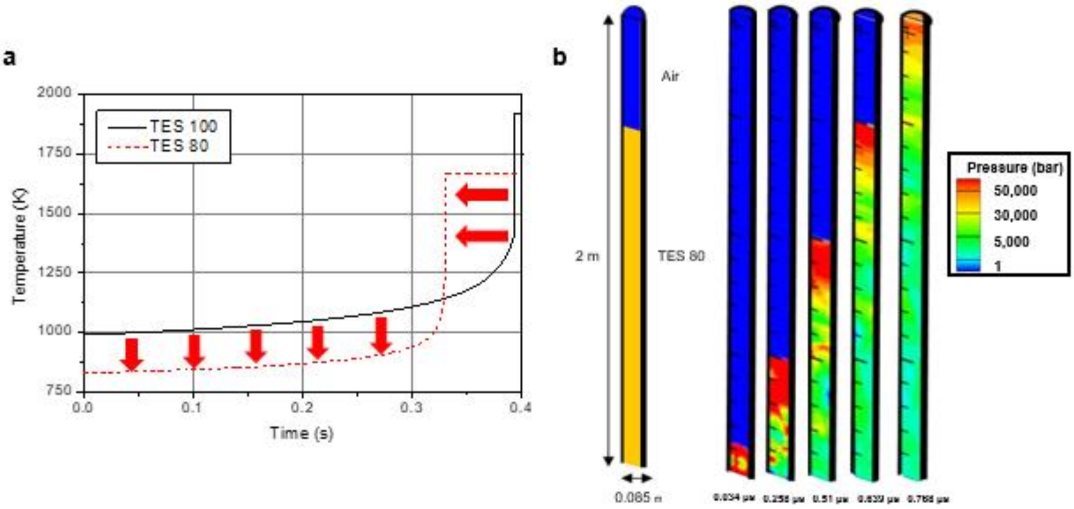


Fig. (a) 0-D simulation based on DSC data and (b) 2-D simulation based on DSC data

담당조교 : 남재현 (wogus1336@snu.ac.kr)

10-3. [수치해석|sim.] Numerical analysis of hypersonic combustion of solid fuel via scramjet combustor (배기훈, Gihoon Bae)

- Solid-gas multiphase reaction in hypersonic combustion of solid
  - Discover the entire mechanism of combustion reaction from polymer chain breaking on fuel surface to gas-phase fuel interaction with heat
  - Capture inner shockwave within the combustor and estimate shockwave effects concerned with combustion
  - Evaluate whether detonation or deflagration wave will take place in the combustor
  - Comparison between solid-fueled scramjet combustor and gas-fueled scramjet combustor in terms of combustion of single-gas-phase combustion and multi-gas-solid-phase combustion of injected fuel

- Simulation of the combustion of solid fuel in the combustor
  - Reynolds Averaged Number Simulation (RANS), k-omega Shear Stress Turbulence(SST) Model on 2-D Simulation for capturing the wall effect on the wall of combustor
  - Large-Eddy Simulation (LES) on 3-D simulation
  - Arrhenius equation based finite-rate chemistry or Flamelet Generated Model (FGM)
  - Case-by-case modeling using both unstructured mesh and structured mesh, or even hybrid mesh
  - Commercial cloud service (i.e. AWS), or parallel computing for large-size simulation

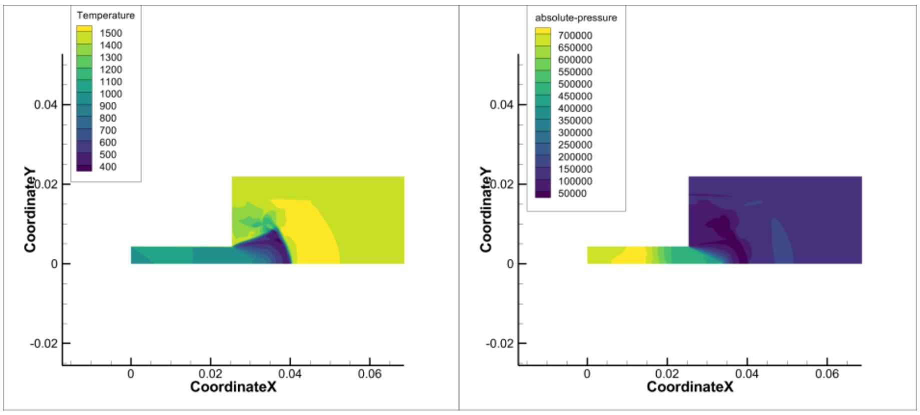


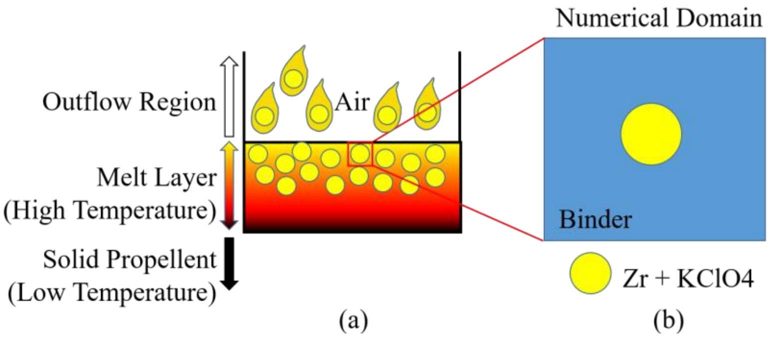
Fig. (a) 2-D Schematic of Temperature Distribution at Combustor Inlet, which captures inner shock in the combustor (b) 2-D Schematic of Pressure Distribution at Combustor Inlet

담당조교 : 배기훈 (10wonsoft@snu.ac.kr)

10-4. [수치해석|sim.] Numerical analysis of metalized solid propellants on the meso-scale (최홍석, Hongsuk Choi)

- Metalized solid propellants
  - High energy density
  - Aluminum, boron, and zirconium …
  - heterogeneous properties because of adding plasticizers and metal particles to change mechanical properties or control the combustion rate

- Numerical analysis
  - Melt layer of Solid propellants on the meso-scale
  - In-house CFD tool called hydrocode using the level-set method and the ghost fluid method



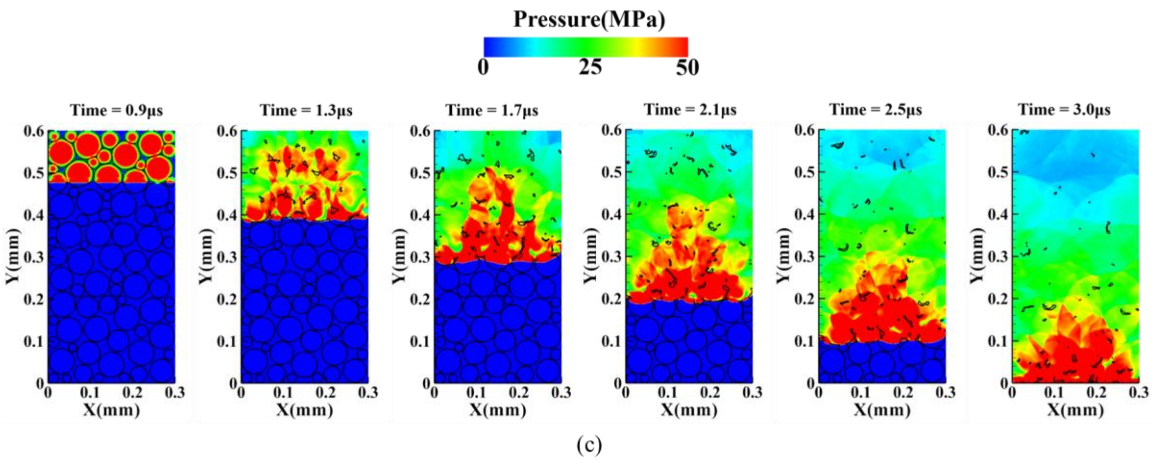


Fig. (a) Schematic of Zr + KClO4 surface burning, (b) Numerical domain, and (c) Zr + KClO4 particle reaction (pressure contour)

담당조교 : 최홍석 (chspider@snu.ac.kr)

10-5. [수치해석|sim.] **Modeling of a long-range high-power laser-artillery shell interaction** (박기성, Kisung Park)

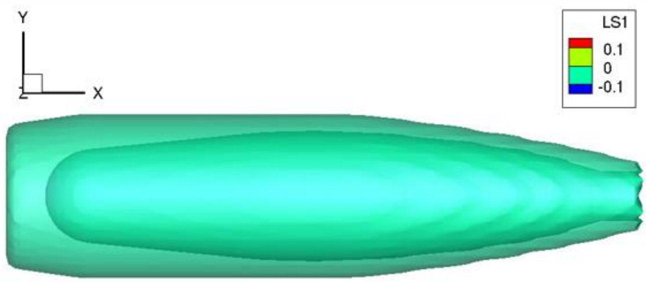
- **Heat transfer effect in metal**
  - When the laser beam is irradiated onto the surface of the shell made of metal, heat transfer occurs due to optical energy.
  - Analyze heat transfer using the heat diffusion equation.

- **Explosion of high-explosive material**
  - As heat transfer increases the surface temperature of the internal material in contact with the metal, the high-explosive material inside the shell explodes.
  - Analyze explosion using compressible Euler equation, Equation of States, and Arrhenius equation.

- **Effects of atmospheric disturbances**
  - Absorption, scattering, refraction, air transmittance, and wind affect the propagation of the laser beam.'

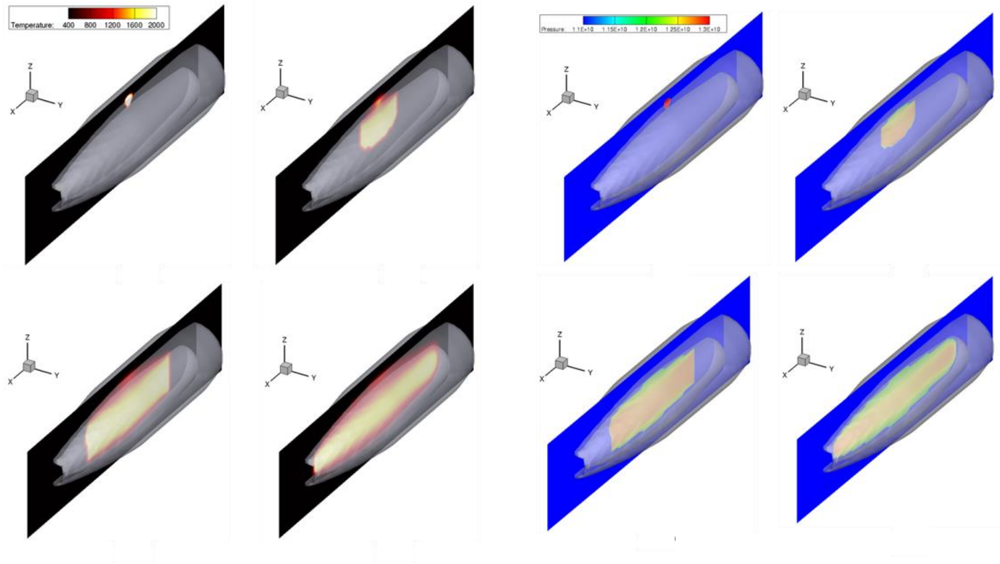
    Analyze the intensity and phase changes of the laser beam using Maxwell's wave equation and equation for calculating phase by thermal blooming.

(a)



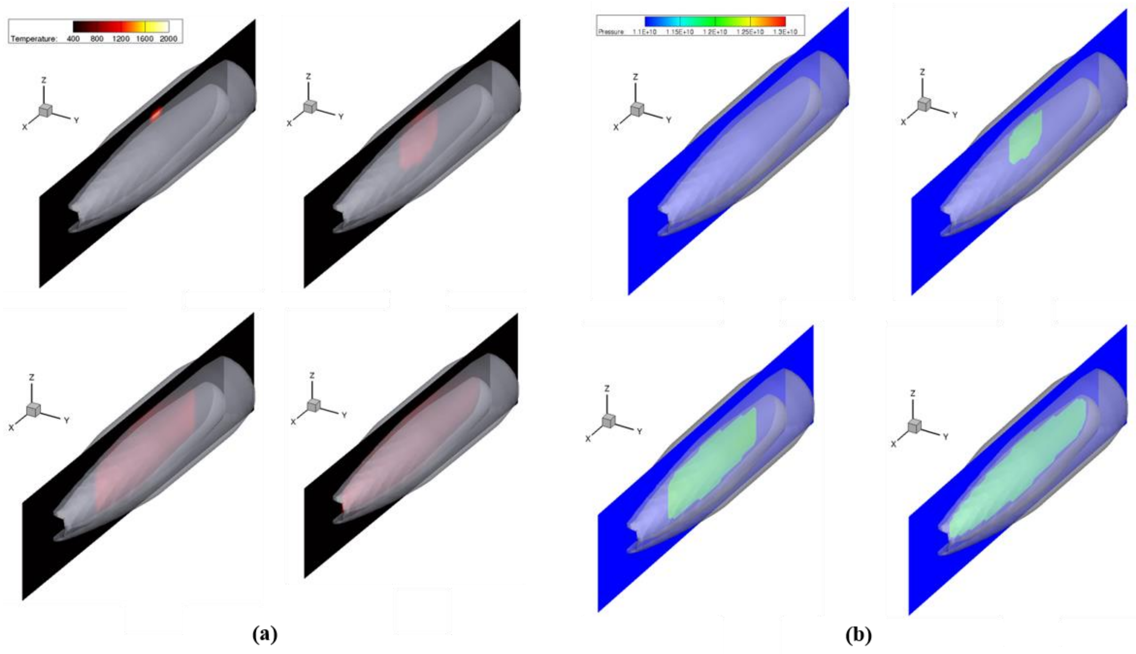
(b)

Fig. (a) CAD modeled and (b) Parameterized level-set of 155 mm shell



(a) (b)

Fig. Simulation result of (a) temperature (b) pressure distribution without atmospheric disturbance



(a) (b)

Fig. Simulation result of (a) temperature (b) pressure distribution with average atmospheric disturbance

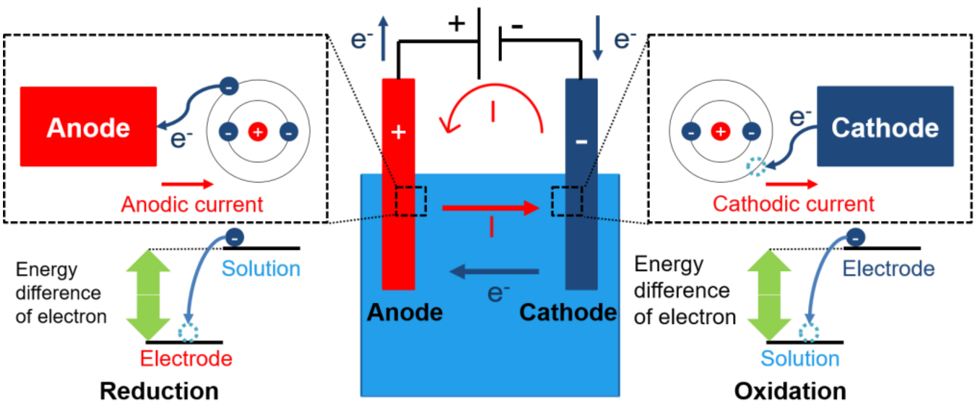
담당조교 : 박기성 **(pac9422@snu.ac.kr)**

10-6. [수치해석|sim.] Numerical Modeling Physical Mechanism of ECSP Combustion

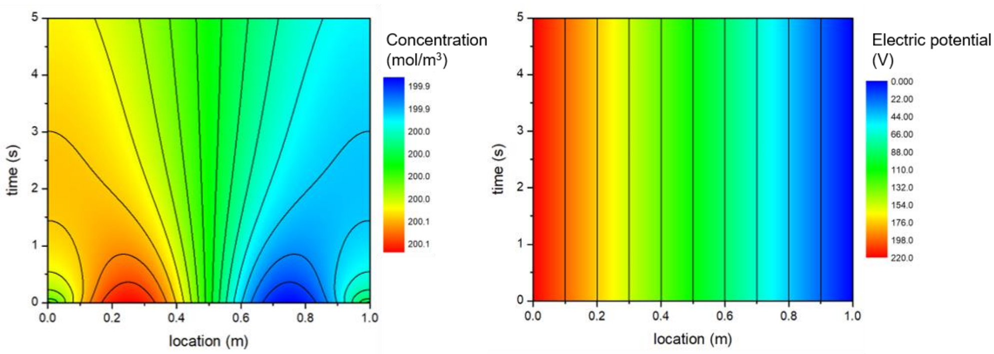
(김민석, Minseok Kim)

- Electrochemistry of Electrically controlled solid propellant
  - Electrochemical system
  - Thermodynamics, electrochemical potential
  - Energy conversion in Electrically controlled solid propellant

- Numerical modeling of ion transfer and electrochemical thermodynamics
  - Development of a solver using Matlab and C language
  - Governing equations of the Electrochemical thermodynamics system
  - Simulation of heat generation by ion transport and chemical reaction



(a)



(b)

Fig. (a) Schematic of interaction with electron, (b) Result contours of 1D ion-transfer model

담당조교 : 김민석 (wayne03304@snu.ac.kr)

10-7. [실험|expt.] Dielectric breakdown-induced shockwave and its biomedical application (함휘찬, Hwichan Ham)

- Mechanism
  - Dielectric breakdown by short pulsed voltage discharging
  - Effective underwater streamer propagation by electron-attractive microchannel

- Shockwave treatment & Medicine injection
  - Application to extracorporeal shock wave therapy (brain-cardiovascular stimulation)
  - Hormonal medicine injection such as insulin, vaccine and antibiotics

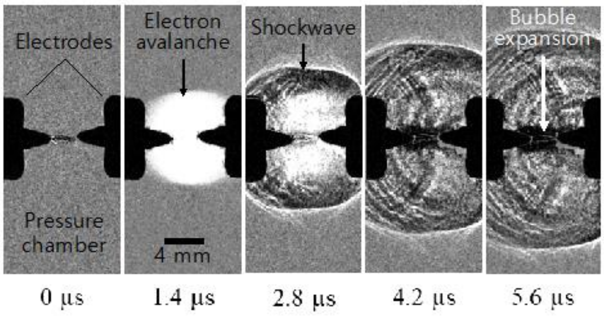


Fig. Pressure contours as per dielectric breakdown

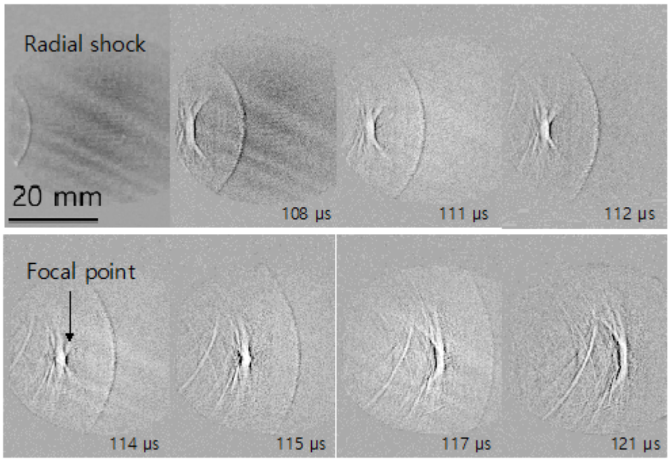


Fig. jet speed and pressure with respect to breakdown voltage

담당조교 : 함휘찬 (hamn2012@snu.ac.kr)

10-8. [실험|expt.] Experimental analysis of combustion behavior of electrically controlled solid propellants (임대홍, Daehong Lim)

- **Combustion dynamics of electrically controlled solid propellant.**
  - Burning characteristics of electrically controlled solid propellants.
  - Analysis of effect of metal additive and applie voltage, etc.

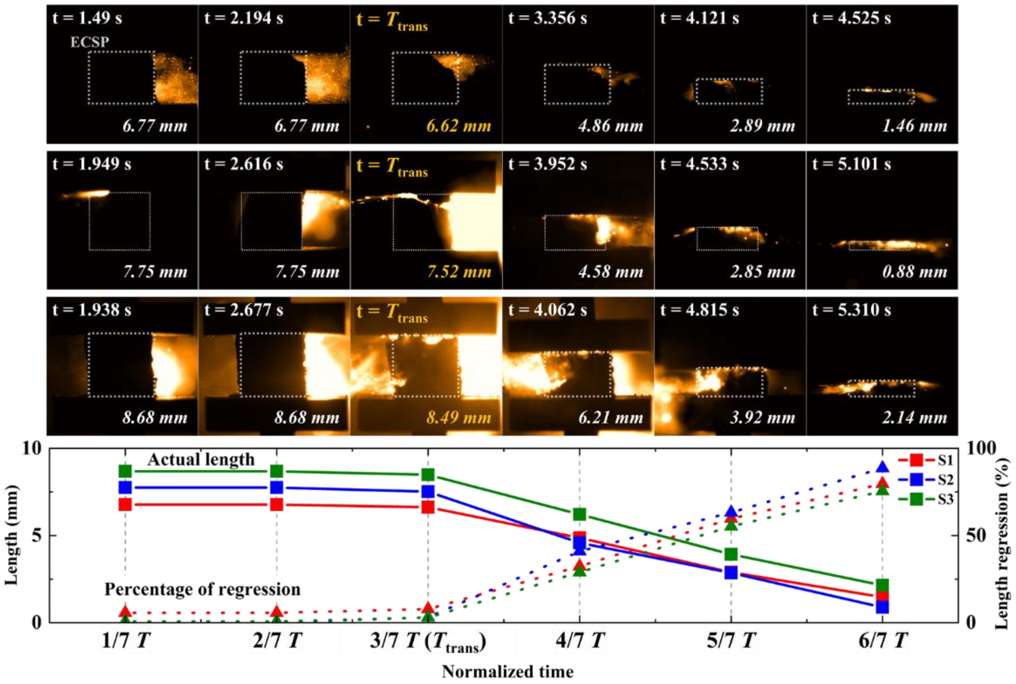


Fig. Burning sequence of the ECSP.

- **Flame visuallization and Diagnostics.**
  - High-speed imaging and laser/non-intrusive diagnostics.
  - Study of the particle-flame interaction.
  - Measurement of the flame characteristics from ECSP.

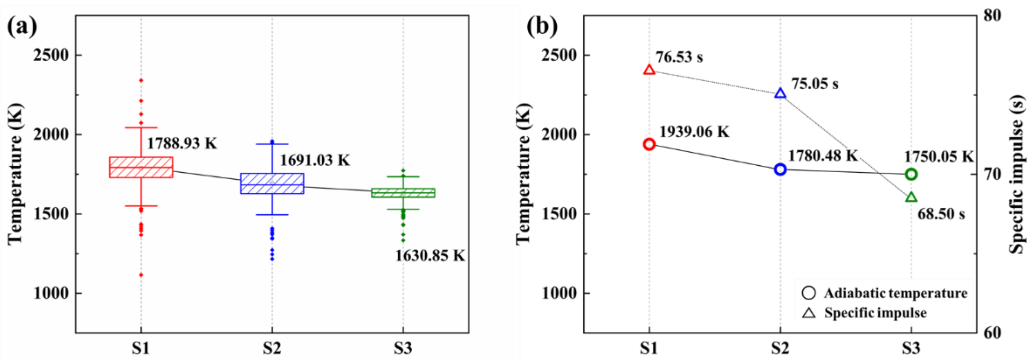


Fig. Temperature measurement and comparison with the theoretical values.

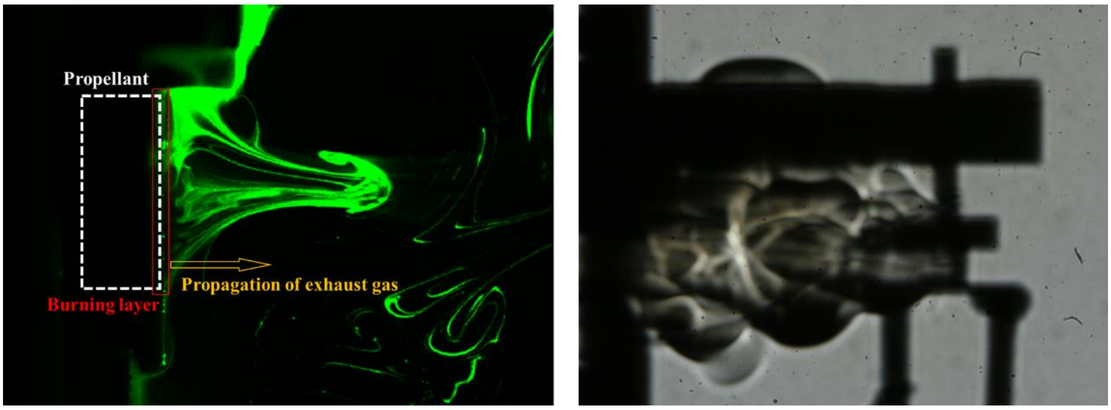


Fig. Visuallized images of flame/exhaust gas.

담당조교 : 임대홍 (**limdae5199@snu.ac.kr**)

10-9. [실험|expt.] **Experimentally understanding the enigmatic combustion of electrically controlled solid propellants** (Rajendra Rajak)

- **Compositional variation effect on the characteristics of the ECSP.**
  - Developing novel ECSP composition.
  - Use of metal additive to enhance ECSP performance.

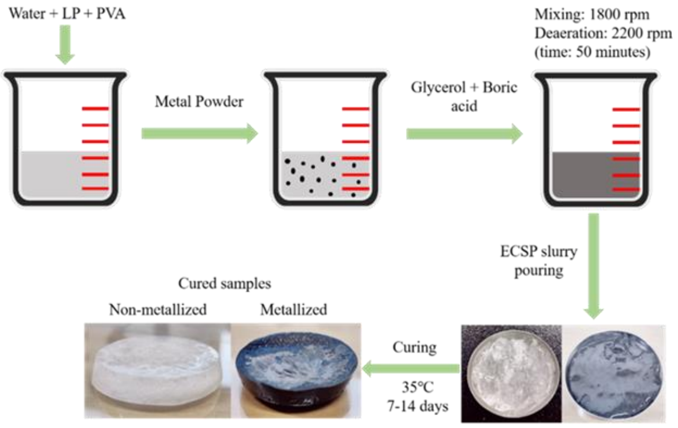


Fig.: ECSP preparation procedure.

- **Implement non-intrusive technique to establish the relation between pressure and regression rates of ECSP with voltage variation.**
  - High speed combustion videography and laser Doppler velocimetry.

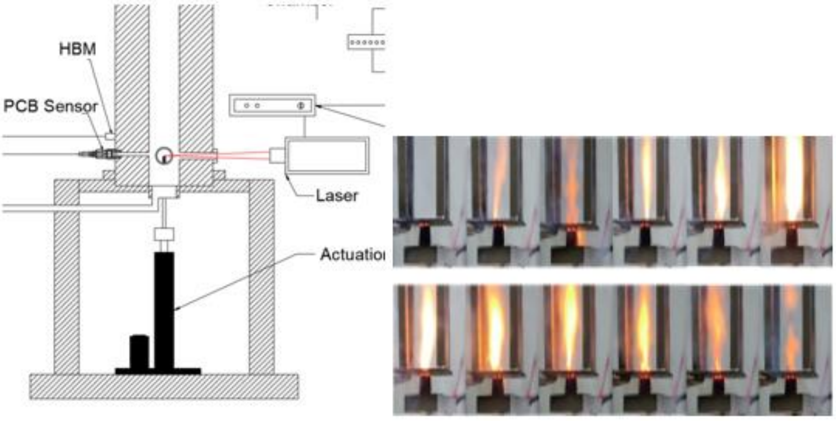


Fig.: Schematic of pressure chamber with LDV focused and atmospheric condition burning images.

- **Small Scale thruster design for micro to macro applications.**

  - Actuation system for continuous thruster operation with feedback mechanism.

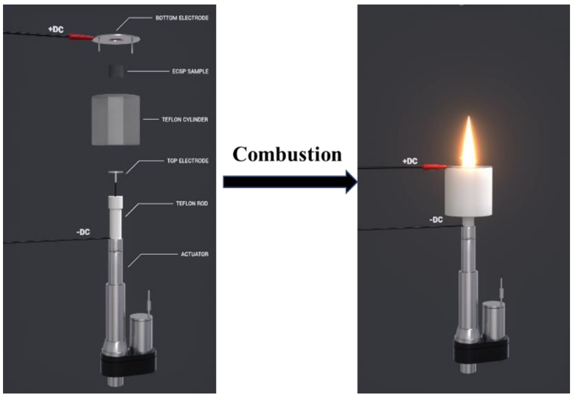


Fig.: Small scale thruster controlled using the actuator with feedback mechanism.

- **Thermal analysis and mass spectroscopy of ECSP to understand the physio-chemical mechanism of ECSP combustion.**
  - DSC, TGA of the novel ECSP compositions.
  - Mass spectroscopy to understand the compositions of the product species.

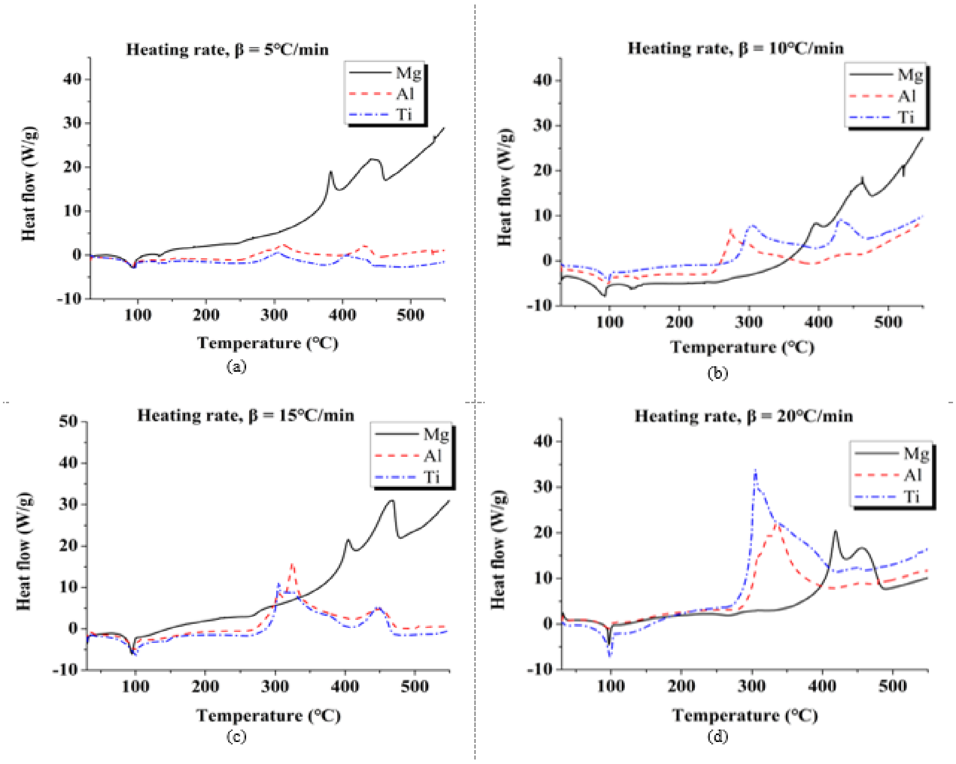


Fig.: (a) DSC curve for Mg, Al and Ti based ECSP at a heating rate of 5 °C/min (b) DSC curve for Mg, Al and Ti based ECSP at heating rate of 10 °C/min (c) DSC curve for Mg, Al and Ti based ECSP at heating rate of 15 °C/min (d) DSC curve for Mg, Al and Ti based ECSP at heating rate of 20 °C/min.

담당조교 : **Rajendra Rajak (Rajendra_rajak@snu.ac.kr)**

10-10. [실험|expt.] Developing a prototype of FEEP Thruster for Nano-Satellite (권찬얼, Chanearl Kwon)

- Field Emission Electric Propulsion (FEEP)
  - FEEP thruster is a form of electric propulsion based on field ionization of liquid metal, and subsequent acceleration of the ions by a strong electric field
  - FEEP thruster has high specific impulse and it is easy to minimize, which is most suitable thruster for nano-satellite
  - There are three different types of emitter (needle, capillary, slit type), and they operate different thrust level
  - In current study, FEEP thruster with annular type slit emitter, which has advantage of higher thrust level and minimizing is presented

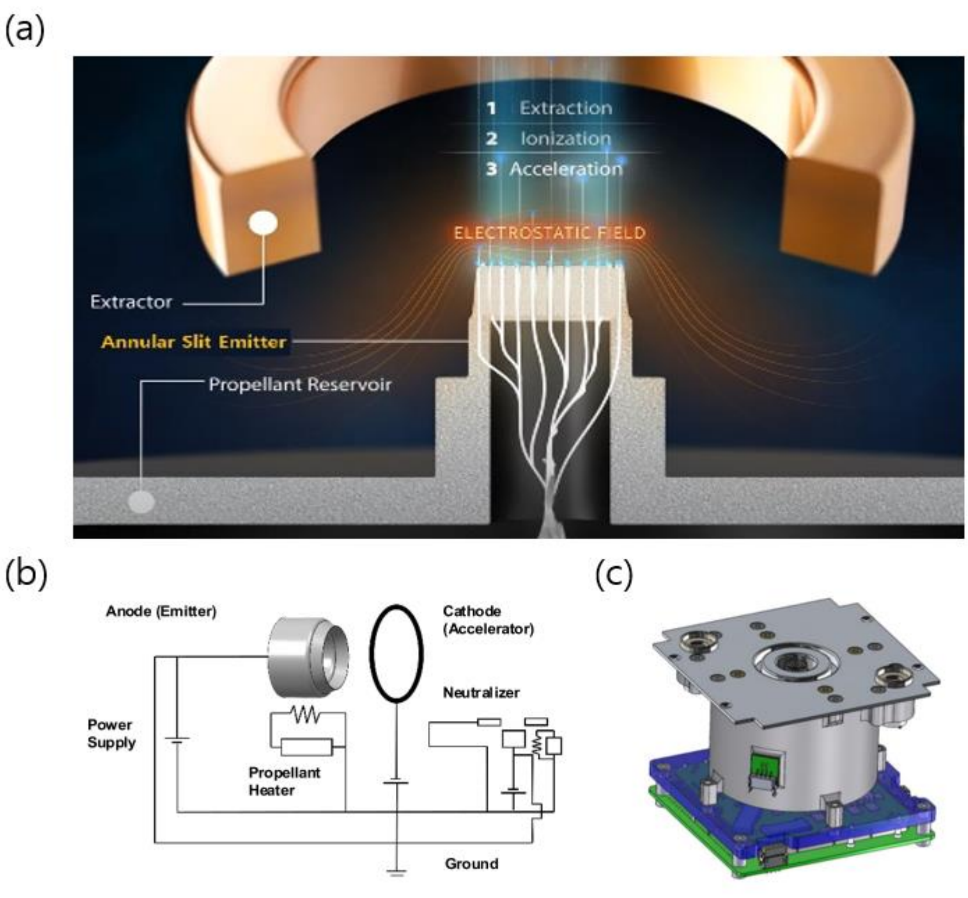


Fig. (a) Visualization of field emission, (b) Electrical schematic of FEEP thruster, and (c) 3D modeling of FEEP thruster

담당조교 : 권찬얼 (rnjscksdjf94@snu.ac.kr)

10-11. [실험|expt.] Aging analysis for the energetic materials comprising of metal fuels (오주영, Juyoung Oh)

- Identification of the effects of the moisture content on the thermodynamic characteristics of the aged energetic materials. (Thermal analysis)
  - Utilized samples: thermally aged or hygrothermally aged metals
  - Instruments: differential scanning calorimetry (DSC)/thermogravimetric analysis (TGA)
  - Thermodynamic characteristics: onset temp., peak temp., endset temp., heat of reaction, peak intensity, peak shape., etc.
  - Kinetic parameters can be calculated by using differential isoconversional method.

- Aging effects on the morphological and structure of the aged energetic materials. (Morphological analysis)
- Measurement of the thermal stability and reactivity in the aged energetic materials. (Combustion analysis)
- Predictions of the lifetime for energetic materials based on metals.

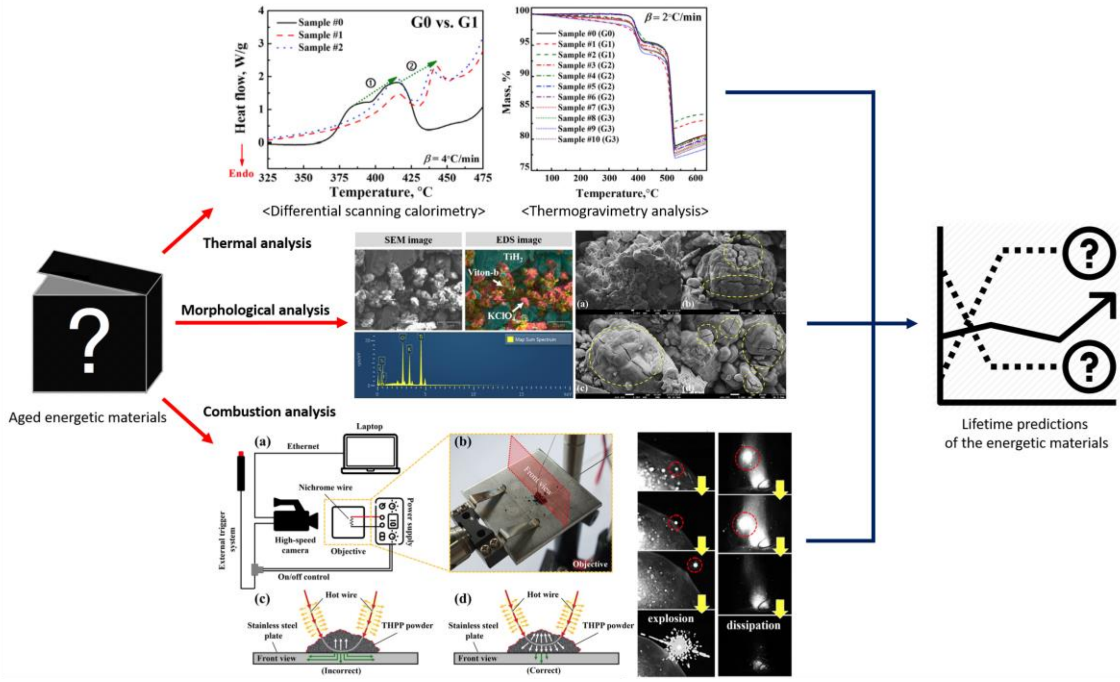


Fig. Illustration of the aging analysis procedure including 'Thermal analysis', 'Morphological analysis', and 'Combustion analysis' for prediction of the lifetime for energetic materials.

담당조교 : 오주영 (5_ju0@snu.ac.kr)

10-12. [실험|expt.] Prediction of thermal runaway characteristics by thermal analysis to secure the battery safety (오주영, Juyoung Oh)

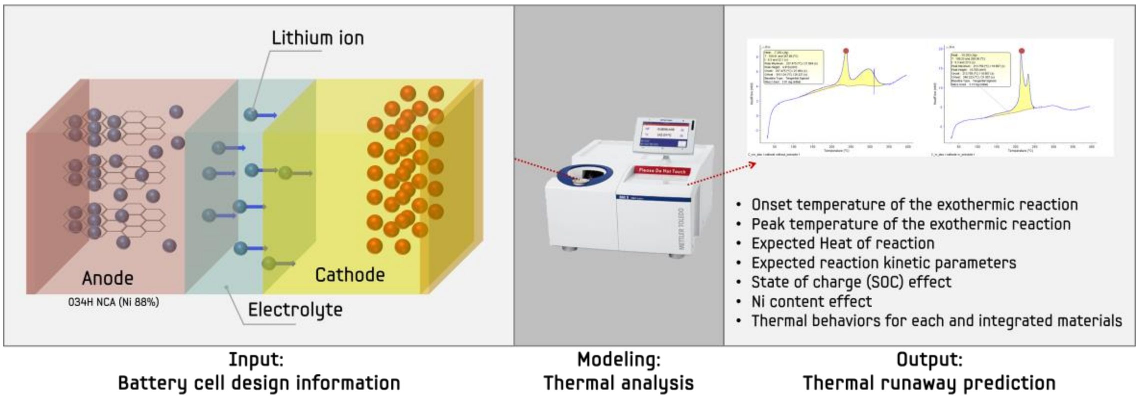


Fig. A flow chart for prediction of thermal runaway of the battery system

- Research objective:
  - Establishment of the prediction model for providing thermodynamic properties with respect to the battery element input.
  - Extraction of the chemical reaction kinetics for each element in the battery cell.
  - Construction of relationship between thermal properties and the battery elements (anode, cathode, and electrolyte) with various state of charge (SOC) or Ni content.

- Experimental approaches:
  - Differential scanning calorimetry (DSC)-Thermogravimetric analysis (TGA)

- Calculation method for extracting the reaction kinetics:
  - Friedman isoconversional method

$$\ln\left[\left(\beta_i \frac{d\alpha}{dt}\right)_{\alpha,i}\right] = \ln[f(\alpha)A_\alpha] - \frac{E_\alpha}{RT_{\alpha,i}}$$

α: Reaction progress, β: Heating rate (K/min), A_α: Pre-exponential factor (1/s), E_α: Activation energy (kJ/mol), T: Temperature (K), R: Universal gas constant (J/mol·K)

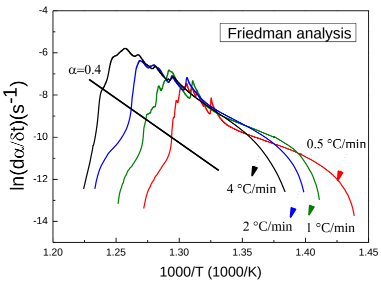


Fig. Friedman isoconversional method (**α**=0.4)

- Predictions of the thermal runaway event of battery cells based on the established models from the thermal analysis.

담당조교 : 오주영 (5_ju0@snu.ac.kr)

10-13. [실험|expt.] Characterization of thermal runaway in ultrahigh-nickel lithium-ion battery from experiments and modelling (우파즈나 Upasana P. padhi)

- Research for
  - High energy lithium-ion batteries (LIBs) with prudent safety measures are key to future transportation.
  - The undesirable thermal events in LIBs can pose a direct risk to battery life and consumers.
  - The attempts to predict the likelihood of thermal runaway in high-energy LIBs have been unsuccessful so far.
- Research Objectives
  - To identifying the thermal events in various active materials used in ultrahigh-nickel LIBs subjected to thermal abuse.
  - To define new criteria to indicate thermal runaway based on rate of heat generation and dissipation
  - Thermal modeling from kinetic analysis.
  - Analysis on vent gases from ultrahigh nickel LIBs to identify the flammability limit and flame speed.
- Experiments
  - Differential Scanning Calorimetry (DSC), Thermogravimetry analysis (TGA) for thermal analysis
  - Gas chromatography and mass spectroscopy (GCMS) for vent gas analysis
  - Kinetic analysis and thermal modeling using MATLAB.

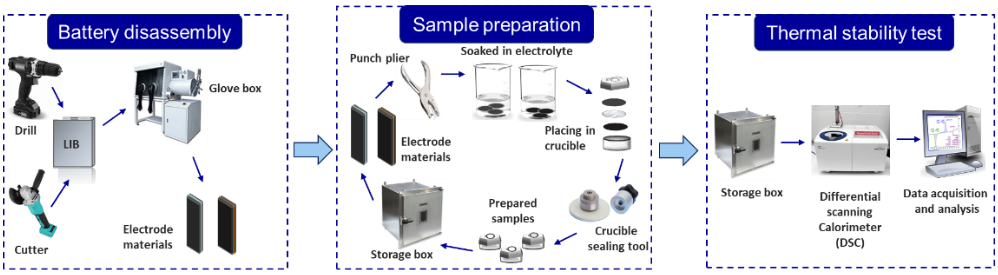


Fig. Sample preparation and experimental settings for thermal analysis of LIB sample

담당 조교 : Upasana P. Padhi (padhi.upasana89@snu.ac.kr), Mehrotra Ayushi (am7997@snu.ac.kr)

10-14. [실험|expt.] Experimental investigation on Taylor cone formation using different emitters for development of FEEP thruster (우파즈나 Upasana P. padhi)

- Research motivation
  - Field emission electric propulsion (FEEP) is deemed the most suitable ion thruster for Nano-satellite's deep space exploration and precision maneuver due to its low thrust and high specific thrust.
  - To understand the basic principle Taylor cone experiment using various types of emitters, ionic liquid ion source for FEEP thruster development.
- Research Objectives
  - To study the Taylor cone formation, cone-jet mode transition in electrohydrodynamics of water, glycerin using capillary and annular type emitters.
  - To characterize the jet formation using various types of emitters, ionic liquid ion source
- Experiments
  - Lab scale Taylor cone generation setup.

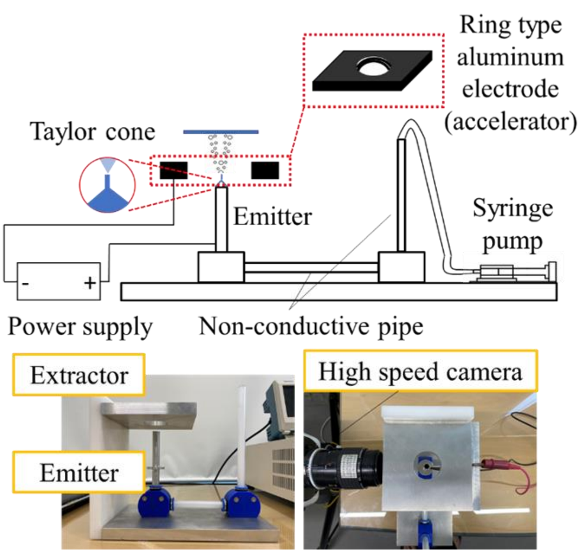


Fig. Experimental Setup for Taylor Cone Formation

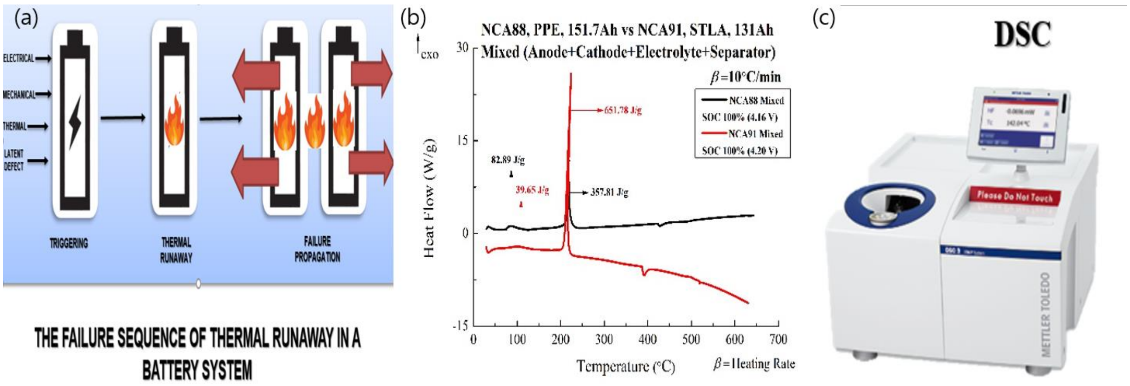
담당 조교 : Upasana P. Padhi (padhi.upasana89@snu.ac.kr), 권찬얼 (rnjscksdjf94@snu.ac.kr)

10-15. [실험|expt.] Comprehensive Study of the Thermal Runaway Characteristics of High-Energy Lithium-ion Batteries using Differential Scanning Calorimetry (DSC) (메흐로트라 Mehrotra Ayushi)

- Research focus:
  - To study the thermal runaway characteristics of High-Nickel, High-Energy Lithium-ion batteries using calorimetry
  - Predict the thermal runaway characteristics of high-energy batteries and identify the conditions that can lead to thermal runaway and failure of the battery
  - Study the thermal runaway characteristics of layered, High-energy battery and identify the effects of layered batteries on thermal runaway phenomenon.

- Research objectives:
  - High-energy battery materials like NCA88/Silicon-carbon composite and NCA91/Silicon-Carbon composite
  - Identify and study the thermal runaway characteristics using Differential Scanning Calorimetry (DSC)
  - Identification of other factors (Layer effect, gas evolution etc.) that can lead to the thermal runaway of high-energy batteries.
- Advantages of High-energy Lithium-ion batteries include:
  - Super-fast charging and long term performance
  - Inherently safer than fossil fuels, excellent and clean source of energy for growing automobile industry
  - Longest life-span, highest efficiency and relatively light and compact compared to other sources of energy, customizable according to energy requirement.
- Experiments:
  - Differential Scanning Calorimetry (DSC) for thermal analysis
  - Scanning Electron Microscope(SEM) for morphological analysis

- Study of kinetic parameters using isoconversional, methods



a) The thermal runaway phenomenon in Li-ion batteries b) DSC results for thermal runaway analysis c) Differential Scanning Calorimeter

담당 조교 : Mehrotra Ayushi (am7997@snu.ac.kr), Upasana P. Padhi (padhi.upasana89@snu.ac.kr)

10-16. [실험|expt.] Thermochemical analysis of magnesium and magnesium-based mixture (이예준, Lee Yejun)

- Research for …
  - How do environmental factors (heat, moisture) and oxygen conditions affect metal fuels?
  - Do magnesium and magnesium-based mixtures have similar trends?

- Objectives
  - Energetic materials (pyrotechnics, propellants, and explosives)
  - Identification of effect of environmental factors (heat, humidity) on metal fuel
  - Identification of influence of oxygen flow rate on metal fuel oxidation

- Metal fuels have many advantages that …
  - High energy density & high specific energy
  - Recyclable
  - No CO_2 emission during oxidation/reduction cycle

- Experiments
  - Differential Scanning Calorimetry(DSC) / Thermogravimetric analysis(TGA) for thermal analysis
  - Scanning Electron Microscope(SEM) for morphological analysis
  - Extracting kinetic parameters by Friedman isoconversional method

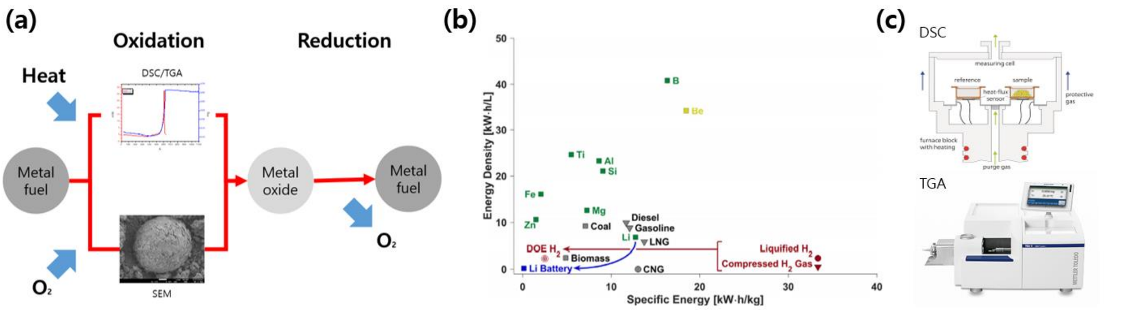


Fig.1 (a) Recycling mechanism of metal fuels (b) Energy density/specific energy of several fuels (c) Experimental equipment (DSC / TGA)

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