



# DISPERSION ANALYSIS AND SIMULATIONS FOR HANDLING OF FUTURE FUELS

**DASH Team**

Vinh-Tan Nguyen © A\*STAR IHPC

7 November 2024

*ARES Confidential*



CREATING GROWTH, ENHANCING LIVES

in collaboration with:



GOVTECH  
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UNIVERSITY  
SINGAPORE

Maritime Energy & Sustainable Development  
Centre of Excellence  
College of Engineering

# Adopting alternative fuels is important in energy transition

## Applications of Advanced Modelling, Simulations and AI for Risk Assessment



The world's first ship-to-container ship bunkering in Singapore, **July 2023**  
First Successful Simultaneous Methanol Bunkering for Container Vessels and Cargo Operation (SIMOPS) , **May 2024**

<https://www.mpa.gov.sg/media-centre/details/singapore-is-ready-for-methanol-bunkering-for-container-vessels-at-tuas-port-with-first-successful-simultaneous-methanol-bunkering-and-cargo-operation>



Suiso Frontier: world's first bulk liquefied hydrogen carrier, **Aug 2023**

<https://www.mpa.gov.sg/media-centre/details/singapore-hosted-the-world-s-first-bulk-liquefied-hydrogen-carrier-suiso-frontier-to-the-port-of-singapore>



Green Frontier: a retrofitted vessel with 4-stroke engine running on a blended ammonia-diesel. Fuel transfer and commissioning, **Feb 2024**

<https://www.mpa.gov.sg/media-centre/details/world-s-first-use-of-ammonia-as-a-marine-fuel-in-a-dual-fuelled-ammonia-powered-vessel-in-the-port-of-singapore>

# Physics of accidental releases and dispersions



## WEATHER & OCEAN

- Weather forecast (NWP, hybrid models)
- prediction of severe events

## SOURCE RELEASE DYNAMICS

- Flashing, phase change, two-phase flows
  - Pool formation and evaporation/revaporisation

## DISPERSION IN AIR

- Dispersion process in O(100s-1000s meters) from sources
- Atmospheric boundary layer (turbulence) effect – thermal stratification

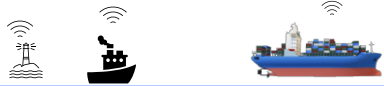
## SENSOR NETWORK

- Fast response and accurate sensors
- Smart sensor network for detection and mitigation

## DISPERSION IN WATER

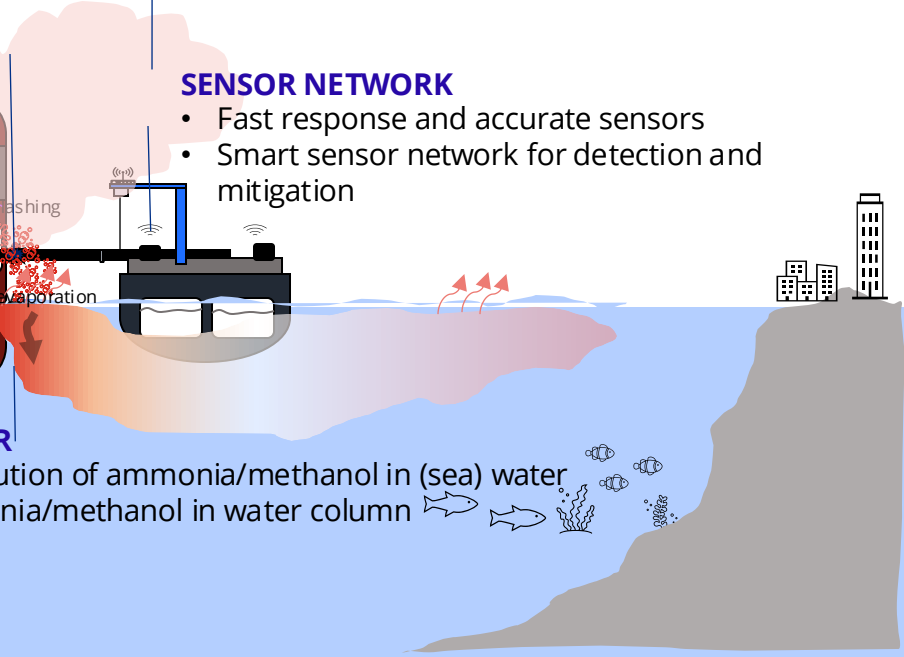
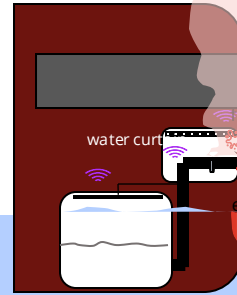
- Solubility and dissolution of ammonia/methanol in (sea) water
- Dispersion of ammonia/methanol in water column

remote sensing



## WEATHER & OCEAN

- ocean hydrodynamic forecast (wind-wave, current + remote sensing)



# Advancing Modelling, Simulation & AI for Safe Adoption of Future Fuels

DASH aims at (1) addressing challenges and gaps in modelling & simulations for risk assessment of future fuel bunkering and (2) translating advances in M&S techniques into operational tools.



Coupled mesoscale with microscale models; coupled atmosphere-ocean-wave model

- Downscaling; coupled surface boundary conditions
- Near-field and far-field coupled model



Two phase release from accidental leakages of liquid fuels

- Phase change, flashing, rain-out from pressurized or refrigerated states
- Solubility of two-phase mixture in (sea) water
- Effects of humidity on buoyant vapour during dispersion process



**Uncertainties** and **accuracy** of multiphysics coupled models for plume dispersion

- Validation of numerical models with experiment and field trials
- Prediction with uncertain environmental conditions (surface layer wind conditions, wave and current)



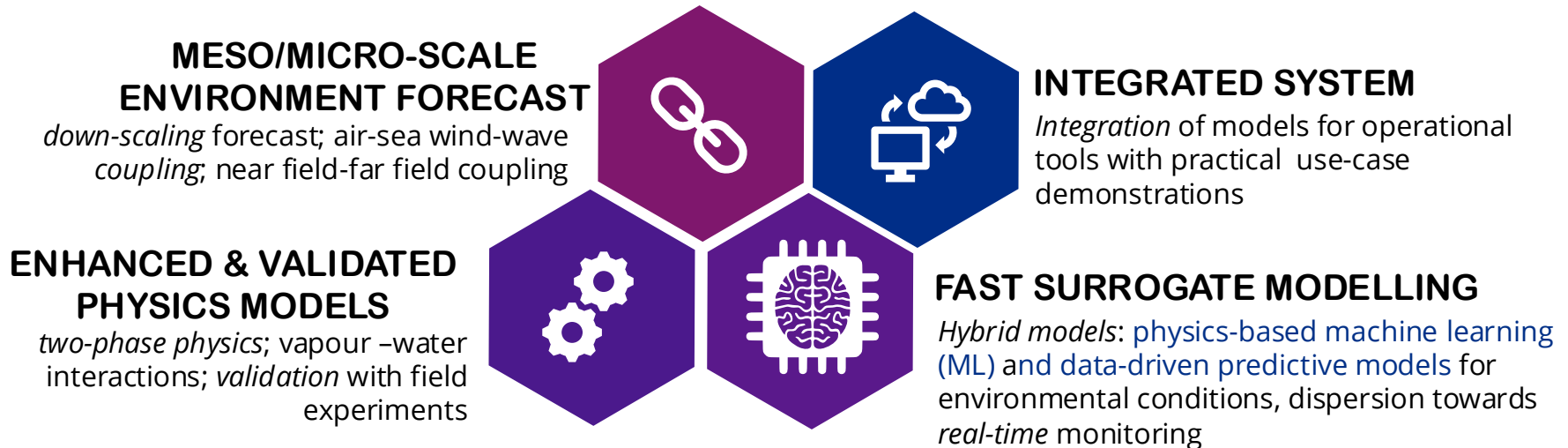
Quick detection of leakages and fast prediction of plume dispersion reducing impacts on human, assets and environment.

- Fast response sensors and robust sensor network to detect leakages
- Fast models for emergency response and preparedness

# DASH: Dispersion Analysis and Simulation for Handling of Future Fuels

Empowering *planning, preparedness, mitigation and emergency response* with model-based decision support system using digital tools developed with advances in

- *Near and far field physics: release sources, dispersion, and consequences coupled with weather & ocean forecast*
- *Accelerated prediction with hybrid physics-based and data-driven surrogate modelling*
- *Validation of models with experiment and demonstration effectiveness of mitigation measures*

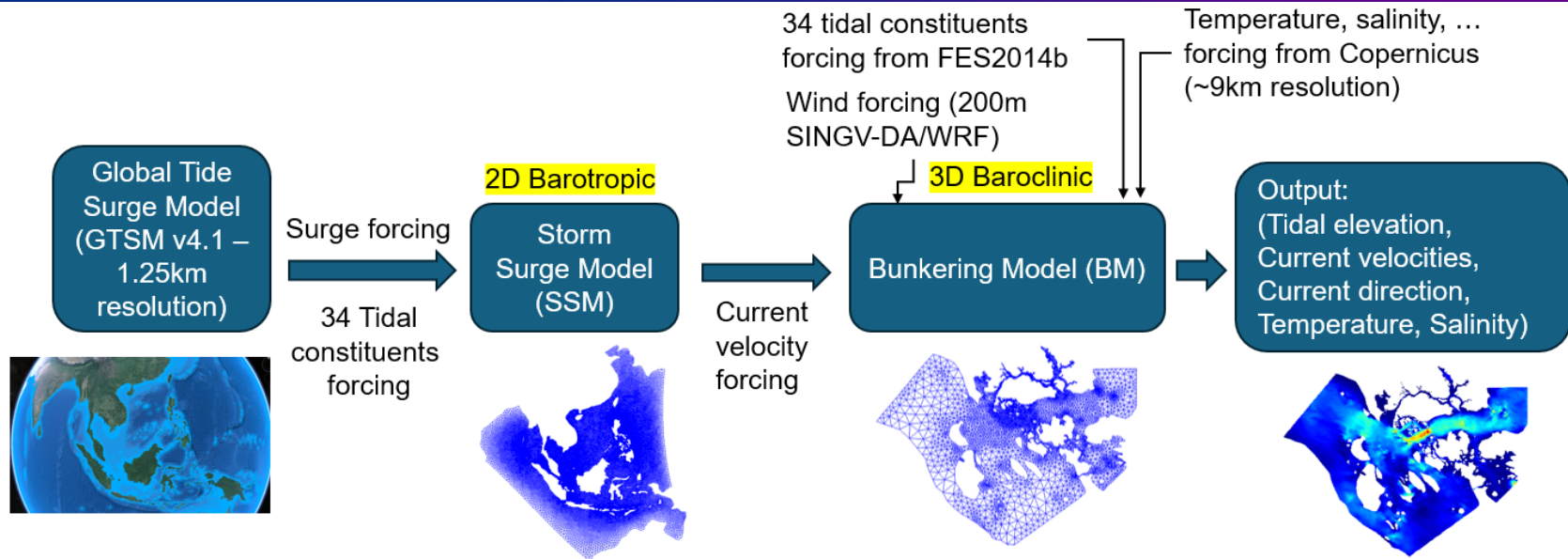


# Coupled mesoscale-microscale forecast of environment conditions

*Developing a suite of models that can be used to dynamically downscale the atmospheric forecasts from the global models to the local Singapore domain.*

*Ocean hydrodynamic forecast from regional to local domain coupled with atmospheric forcing for predictions of tide and current in Singapore strait and beyond*

*Data assimilation techniques to enhance performance of local models for forecasting of environment conditions*

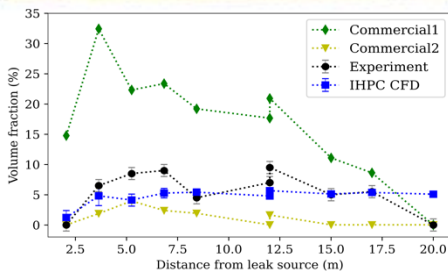
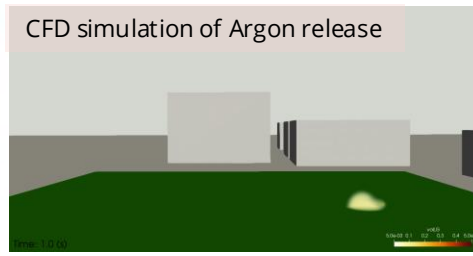


# Enhancing model accuracy with multiphase and coupled physics for plume dispersion simulations

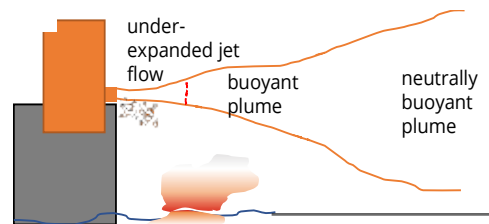
Advanced models for two-phase release providing more accurate prediction of vapour plume dispersion

Coupled weather and hydrodynamic forecast with dispersion in air and dissolution in water for comprehensive consequence analysis of accidental releases.

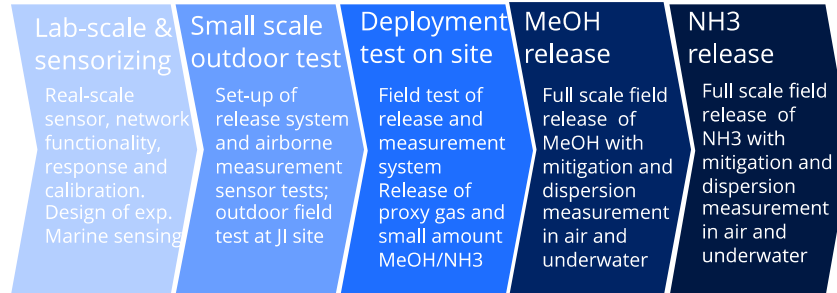
Validation of models with lab-scale and field release experiment for accuracy and uncertainty quantification



Validation and benchmark of CFD model



Two-phase release of ammonia/methanol over sea surface



Phase-gated field experiment campaign for validation of developed models

- Release over (sea) water surface
- Dispersion both in air and water column
- Effects of local climate conditions

# DASH: Comprehensive verification and validation to quantify *uncertainty* and *sensitivity* in prediction

Tapping on existing/available data and future experiment to comprehensively validate models developed in DASH programme

- Quantifying model errors, uncertainties (epistemic vs aleatory)
- Reports and documentations

## Observational Data

### **Existing weather station (AWS)**

Data from 24+ stations across the island for validation/benchmark of atmospheric forecast model

### **Tidal Gauges, ADPC**

Current and wave monitoring stations around Singapore for validation of hydrodynamic forecast models

### **Onsite sensors (MESN, NEPTUNE, etc)**

Both surface wind + hydrodynamic monitoring for validation of near field wind map, hydrodynamic models

## Experiment Data

### **ASTI experiment** (MESD/IHPC [TBC])

ammonia release on land, release under water.

### **Post release impact and mitigation evaluation** (LCER2 funded):

lab-scale experiment for ammonia absorption and mitigation effectiveness

### **Texas A&M Experiment [TBC]**

(TAMU/ABS/IHPC/MESD): lab-scale controlled experiment for ammonia

### **Literature database**

## Field Release Exp

### **WP5: controlled release of ammonia and methanol:**

Field release of ammonia/methanol in tropical climate for validation of developed models

Local experiment with tropic conditions

**Chemspill exercises:** releases of proxy liquids and collecting data for validation of models + testing of monitoring and mitigation technologies (drones, water spray)



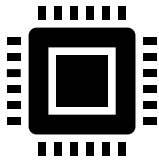
# DASH: Translating advances in modelling and simulations into operational outcomes for future fuel handling



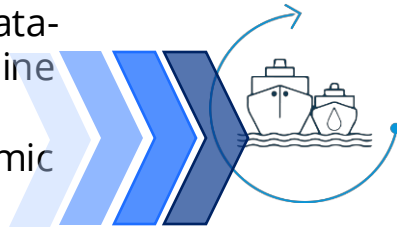
**Validation** of the developed models with experiment; **benchmark** with existing tools commonly used in the industries.



Integrated tools for capacity & operational planning, incident management & emergency response



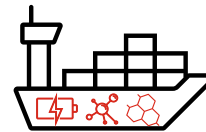
**Acceleration** prediction with data-driven and physics-based machine learning surrogate models for localized weather & hydrodynamic forecast, plume dispersion



Future *bunkering trials, chemspill exercises* as live test best for demonstration of capabilities



**Coupling and integration** of **models** for risk assessment and development of effective mitigation measures



Industrial use-cases: Newly designed and built alternative fuel powered vessels, Proof-of-concept tools for commercialization

## Translatable Outcomes

# Outlook

Atmospheric and ocean forecast coupled with environmental impact assessment

- **Assessment and identification potential bunkering sites**

Understanding and modelling complex physics associated with pressurized or refrigerated alternative fuels upon release into environment

- **Phase change and two phase release: flashing, rain-out**
- **Solubility of two-phase mixture in (sea) water**

Fast detection and subsequent response to accidental leakages reduces impacts on human, assets and environment.

- **Fast models for emergency response and preparedness**

## Our Research Partners and Collaborators





POWERING DISCOVERIES



THANK YOU

for your attention