Green Marine

Retrofitting towards climate neutrality

Development of a standalone thermodynamic property package for the simulation of flue gases with COBIA

30 October 2025

Dimitrios Sykas, Iraklis Lazakis

Funded by the European Union

Green Marine is funded by the European Union funding from the European Union's Horizon Europe research and innovation program under grant agreement No. 101096522. UK participants in Horizon Europe Project Green Marine are supported by UKRI grant numbers 10064539 (University of Strathclyde), 10068477 (CalMac Ltd) and 10064666 (CCM).

Outline

Green Marine

- Speaker Introduction
- First contact with CAPE-OPEN (the Green Marine Project)
- The problem
- Thermo Package Overview
- Overall experience with COBIA

Speaker information

Second year PhD candidate, dept. Naval Architecture, Ocean & Marine Engineering (NAOME)

University of Strathclyde, Glasgow

PhD topic: Cryogenic carbon capture for maritime applications

M.Eng. in Naval Architecture and Marine Engineering

National Technical University of Athens, Greece

Diploma thesis on cryogenic tank modelling

Areas of interest: Systems modelling, Thermodynamics, Computer Programming

CO-LaN Individual Member since July 2025

First contact w/ CAPE-OPEN: The Green Marine project

- EU/UK funded project
- Duration: 4 years (Feb. 2023 — Jan. 2027)
- 10 partners across Europe and UK
- Addresses the development and testing of CO2 emission reduction technologies for marine use
- Website: https://greenmarine-project.eu/
- LinkedIn: https://www.linkedin.com/company/green-marine-project

Current status

- ✓ Lab-scale testing: **complete**
- ✓ Workshops w/ overseeing classification society (Lloyd's Register): **complete**
- ⏱ Addressing LR comments: **ongoing**
- ⏱ UK Maritime and Coastguard Agency consultation: **ongoing**
- ⏳ Land-based testing of integrated carbon capture and emission reduction module: **in the next 2-3 months**
  - Onboard demo to follow

Project partners

Green Marine

CalMac Ferries Limited

Ship Owner

CYPRUS MARINE & MARITIME INSTITUTE

Testing Site

SINTEF

CC through
Membrane Separation

CCM
the carbon capture machine

CC through
Chemical Absorption

SMP
Smart Material Printing
The next step in 3D Printing

WindplusSonne

Pre-treatment & Air reuse

PDM

Technology catalogue tool
&
Retrofitting protocols

University of Strathclyde Glasgow

Onboard installation &
Dissemination

BlueXPRT
Realizing Innovations

UNIVERSITÀ POLITECNICA DELLE MARCHE

LCA, TEA assessments

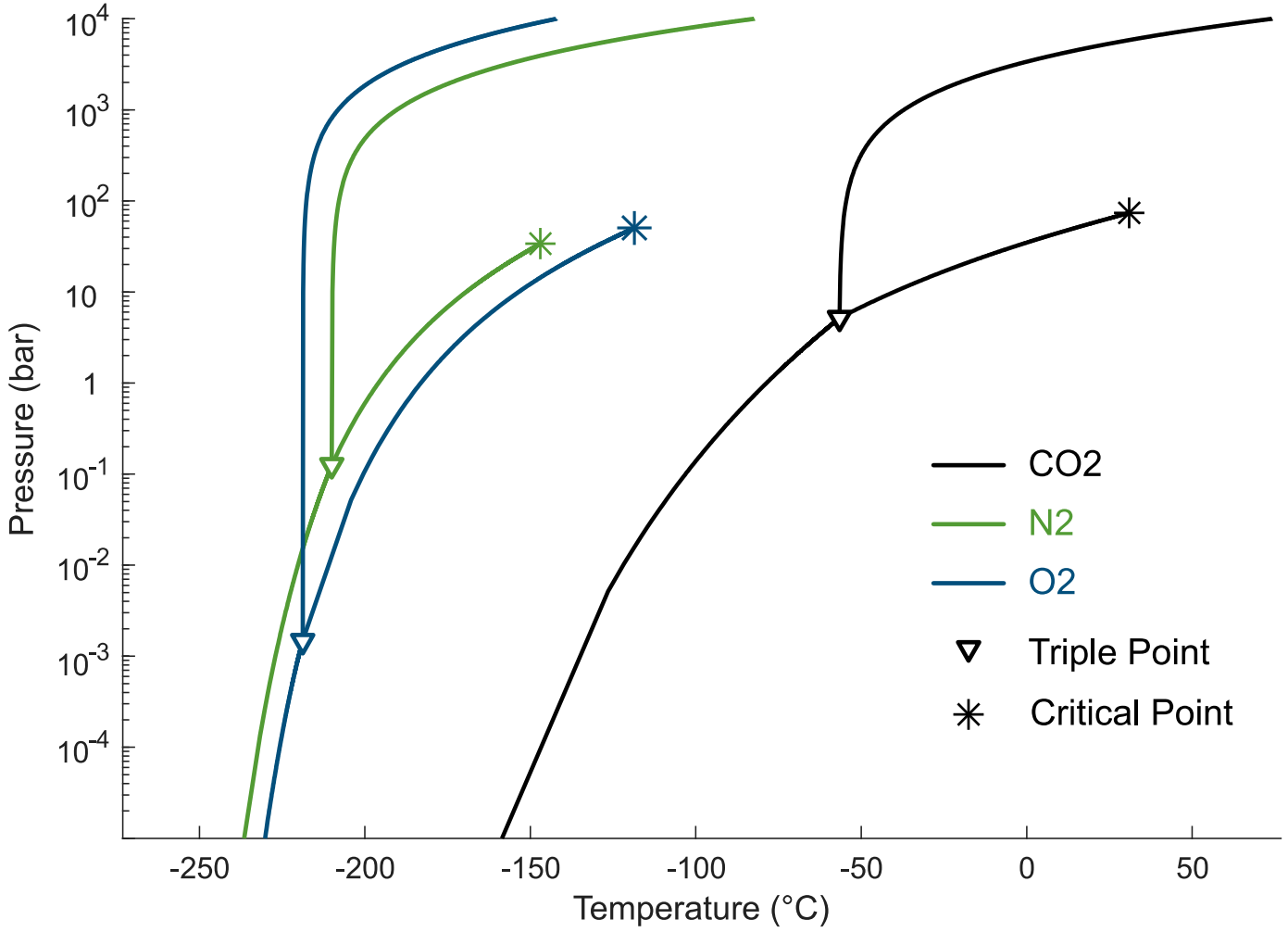
The problem or: why I need a custom Thermo Package

PhD topic:

Modelling and Optimisation of Cryogenic Carbon Capture systems for maritime applications

Challenges:

- Modelling CO2 desublimation
- Using the model in simulations
- Sharing the simulations



Modelling CO_2 desublimation

- No commercial property package with in-built support for solids
- Solid-Fluid Equilibrium calculations?

→ Possible with Aspen's RGibbs unit operation

However…

- RGibbs only works at constant Temperature, Pressure
- Use of Aspen Plus required (licensing/access issues)
- Limited to equations of state already present in Aspen

→ What about the properties of solid CO2?

- What if I wanted to share the model?

Modelling CO_2 desublimation

The solution?

Development of a CAPE-OPEN (CO) compliant thermodynamic property package

Fluid phases: REFPROP

- Highly accurate EoS (GERG-2008, PR w/ BIP)
- Flash calculations (two-phase)
- C++ API

Solid phase: Jäger-Span EoS

- Gibbs free energy-based EoS
- Pure CO2 assumed
- Non-constant volume

Thermo-Package Overview

Uses COBIA middleware

CAPE-OPEN Thermo v1.1

- ICapeThermoCompounds
- ICapeThermoPhases
- ICapeThermoPropertyRoutine
- ICapeThermoEquilibriumRoutine
- ICapeThermoMaterialContext
- ICapeThermoUniversalConstants

Common Interfaces

- ICapeIdentification
- ICapeUtilities
- ICapePersist

Thermo-Package Overview

Uses COBIA middleware

CAPE-OPEN Thermo v1.1

- ICapeThermoCompounds
- ICapeThermoPhases
- ICapeThermoPropertyRoutine
- ICapeThermoEquilibriumRoutine
- ICapeThermoMaterialContext
- ICapeThermoUniversalConstants

Common Interfaces

- ICapeIdentification
- ICapeUtilities
- ICapePersist

ICapeThermoPropertyRoutine

Inputs are mostly `CapeString` strings.

REFPROP works with `std::string`

- Assign `CapeString` to a temporary `CapeStringImpl` variable
- Try to match the `CapeStringImpl` to an enumerated value
- Implement lookup table for matching the enum to REFPROP input

ICapeThermoPropertyRoutine

What about derivative support?

REFPROP provides some:

- T, P, D: all pairings, up to 2nd order
- H, S: with regard to T, P, D (with either one of the remaining properties constant)

What about (log-)fugacities and other properties though?

Implementing per-case derivatives would be messy…

Instead: Implement common 4th order finite difference method

ICapeThermoEquilibriumRoutine

Green Marine

Everything is delegated to REFPROP

Input could be used as-is, except of `specification` strings

For fluids, valid input specifications are:

- Any combination of: T, P, D, E, H, S, Q (vapor fraction)

Calculations involving solids not yet implemented.

CO & REFPROP Compatibility

REFPROP only accepts normalised input

The CAPE-OPEN (CO) standard allows non-normalised compositions

1. Check input
2. Normalise if needed
3. Update material with normalised composition

> argument must be equal to the number of Compounds in the Material Object. It should not be assumed that the mole fractions are normalized and values may also lie outside the range 0 to 1. If fractions are not normalized, or are outside the expected range, it is the responsibility of the Property Package to decide how to deal with the situation.

Excerpt from the CO Thermo 1.1 specification document

my first big C++ project :)

My COBIA experience

Green Marine

Majority of issues not COBIA-specific, rather C++ related

linking, include hell, necessary undefine statements, debugging

COBIA-specific troubles boil down to the lack of documentation:

- Proper usage of `Cape[Type]`, `ICape[Type]`, `Cape[Type]Impl` and especially, `CapeString`
- How to use `CapeSimulationContext`?

Developing a property package is more involved than I expected

(I had been warned!!!)

My COBIA experience

Overall:

Custom types are confusing

but...

COBIA seems better than the alternatives (COM)

Bottom line:

I would happily use it again in future projects

My COBIA experience

For future reference:

- Documentation with sample code will be necessary
- The `PropertyTester` Unit Operation was very useful for debugging

  ...I would like to see it incorporate more tests
- I'd like to see wrappers for .NET languages too

Q&A

dimitrios.sykas@strath.ac.uk

https://pureportal.strath.ac.uk/en/persons/dimitrios-sykas

Debugging issues

The error message buffer is not large enough sometimes…

```
removed property dewPointTemperature
removed property dewPointPressure
added property bubblePointTemperature
added property bubblePointPressure
added property dewPointTemperature
added property dewPointPressure
warning: Material object error in CalcEquilibrium: CalcEquilibrium failed: CalcEquilibrium failed: in ICapeThermoEquilibriumRoutine::CalcEquilibrium of CCC Thermo: Temperature-phaseFraction flash failed: [TQFLSH error 121] Temperature inp
Loaded CHP.fsd
warning: mole fractions for material 1 do not sum up to unity (3x)
```

Workaround: Get error message from COLTT

However, sometimes:

- "Error reading file"

strange but ok, COLTT files are plain text anyway

- COFE crashes when COLTT is attached to certain Uos (e.g. Flash Column)

no idea what causes that…

The PropertyTester UO

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O
34	virialCoefficient										Failed to calculate property: GetTDependentProperty fa				
35	viscosityOfLiquid										Failed to calculate property: GetTDependentProperty fa				
36	viscosityOfVapor										Failed to calculate property: GetTDependentProperty fa				
37	volumeCh	N/A	N/A	N/A							Values are missing				
38	volumeCh	N/A	N/A	N/A							Values are missing				
39	volumeOfLiquid										Failed to calculate property: GetTDependentProperty fa				
40	volumeOf	N/A	N/A	N/A							Values are missing				
41															
42	Exported F	boilingPointTemperature, meltingTemperature													
43															
44	property	carbon di	dinitroger												
45	boilingPointTemperature												property: GetPDependentProperty fa		
46	meltingTemperature												property: GetPDependentProperty fa		
47															
48	----------														
49	1-PHASE PROPERTIES														
50	----------														
51															
52	Exported s	activity, activityCoefficient, compressibility, compressibility.Dtemperature, compressibility.Dpressure, compressibility.Dmoles, compressibilityFacto													
53															
54	property	type	[carbon di	[dinitroge	[dioxygen]	d [carbon	d [dinitrog	d [dioxyge	d [carbon	d [dinitrog	d [dioxyge	d [carbon	d [dinitrog	d [dioxyge	d [carbon	d
55	activity(Va	intensive	1.01563	1.01371	1.01385				1.32E-05	2.20E-06	3.16E-06				1.00E-05	
56	activityCo	intensive	6.77088	1.44816	6.759				8.79E-05	3.15E-06	2.11E-05				6.67E-05	
57	compress	intensive	9.87E-06			-3.87E-11			-3.87E-11			-9.74E-11			-9.74E-11	
58	compress	intensive	1.00001			3.93E-06			3.93E-06			9.49E-11			9.49E-11	
59	density(Va	intensive	30.4662			-0.07629			-0.07628			0.000301			0.000301	
60	enthalpy(	extensive	13845.6			31.2224			31.2226			-5.16E-05			-5.16E-05	
61	enthalpyN	extensive	13845.6			31.2224			31.2226			-5.16E-05			-5.16E-05	
62	entropy(Va	extensive	198.72			0.078056			0.078053			-8.22E-05			-8.22E-05