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Final conference

Modelling VLSFO weathering

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Marine Forecasting Centre
https://www.marineforecasts.be/

Malta, 31/05/2022

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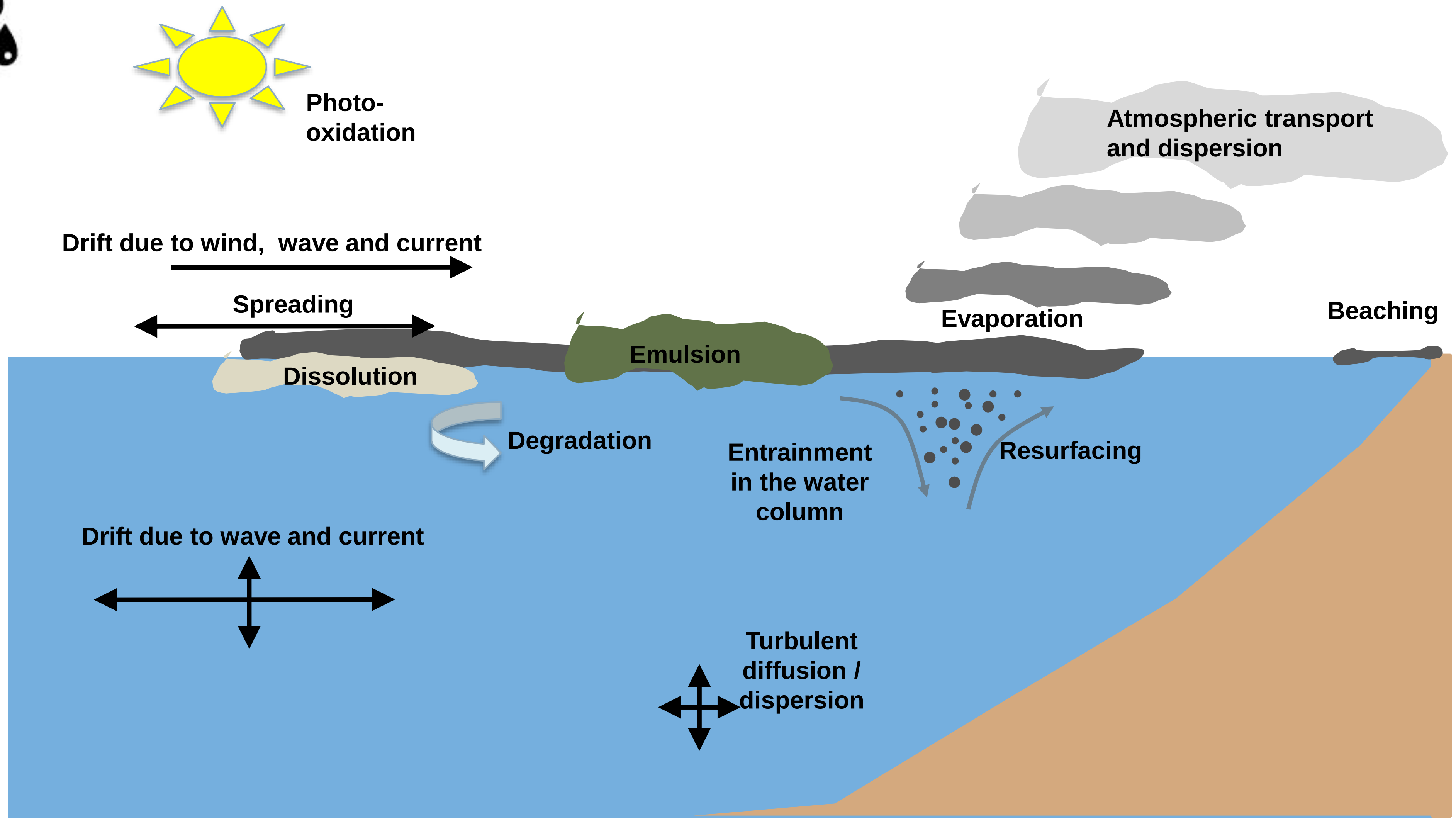

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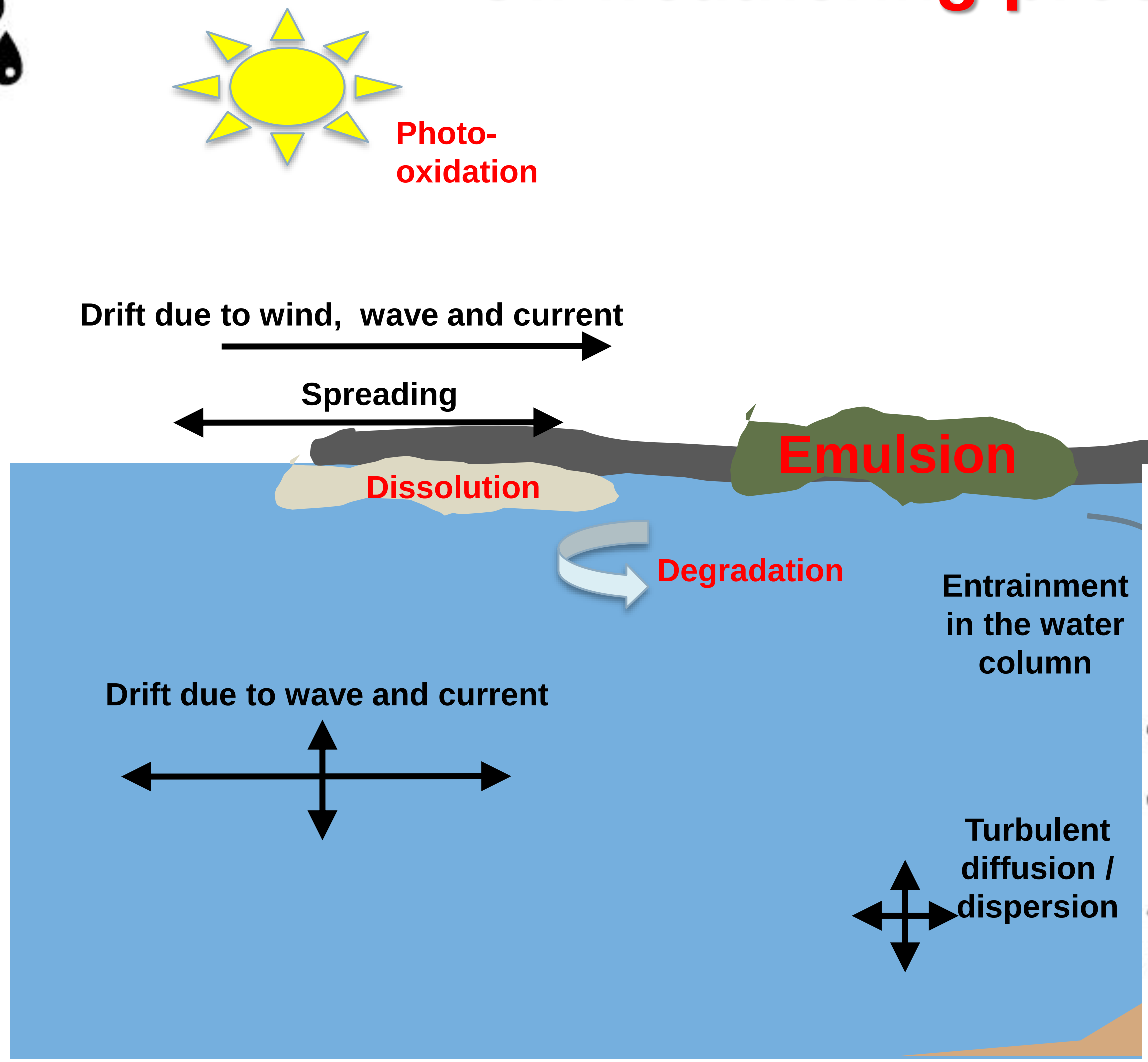
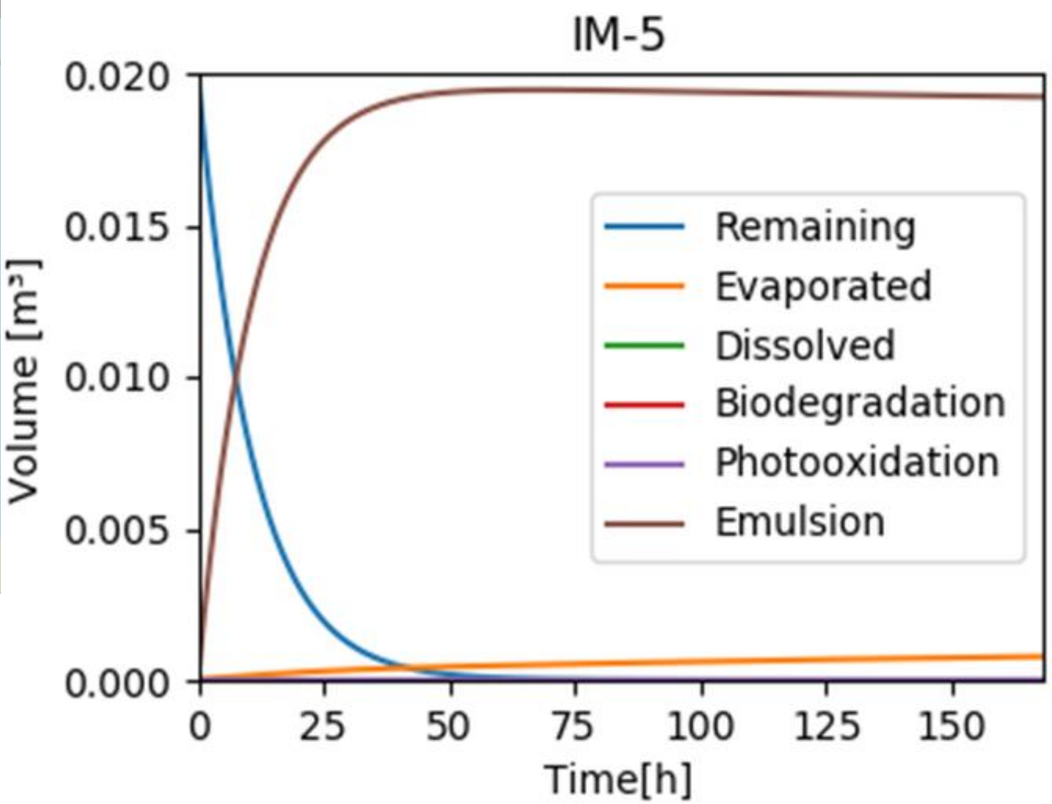
Oil weathering processes





Are the existing parameterizations able to simulate VLSFO weathering?

Can you trust in oil weathering model forecast for VLSFO?

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Validation/invalidation exercise

Weathering model vs polludrome data

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A "toy" weathering model

Evaporation

- Lyman/Jones (as in Oiltrans)
  - Temperature
  - Wind speed
  - Slick length
  - Molar volume
  - Schmidt number in air
  - Vapor pressure
- Brighton (as in ALOHA)
  - Stability class
  - Wind speed
  - Slick length
  - Molar weight (for molecular diffusivity)
  - Vapor pressure
- Fingas (as in OSERIT)
  - 2 empirical constants

Emulsification

- Scory (as in OSERIT)
  - Wave height
  - Kem
  - C
  - Maximum water content
- Mackay
  - Wind speed
  - Maximum water content
  - C

Volatilization : Lyman

Dissolution : Mackay and Leinonen

- Solubility
- Molar volume (for diffusion coefficient)
- Windspeed
- Water volume

Photooxidation

- Half life constant

Biodegradation

- Half life constant

Density

- Evap
- Dissolution
- mulsification

Viscosity : Betancour

- Temperature
- Evaporation
- Emulsion

GitHub https://github.com/naturalsciences/weathering_module_4_marine_pollution

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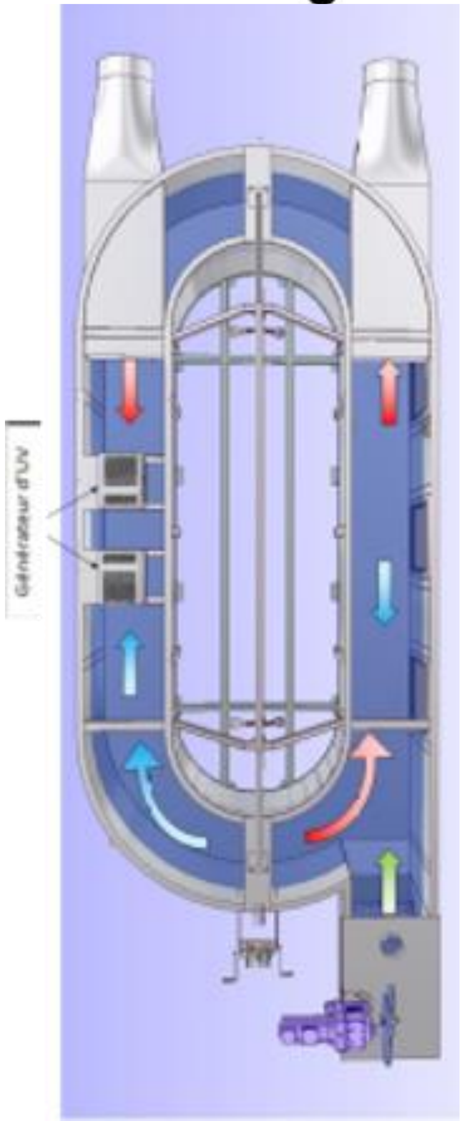
Experimental set-up
Cedre's polludrome



Polludrome geometry

- Sea water volume : 7 m³
- Sea water depth : 0,9 m
- Polludrome surface : 7.78 m²

Controled 'enviromental' conditions

- Wind : 5m/s
- Currents : 0,4m/s
- Waves height : 0,75 m
- Air temp : 15°C
- Sea water temp : 15°C

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Lab characterization of benchmarked oils at 15°C

Fresh oil (covers Density through Pour point rows)

At 15°C	IM-5	IM-14	IM-15
Density [kg/m³]	909	937	951
Viscosity (10s^{-1}) [mPa s]	3051	17121	4305
Viscosity (100s^{-1}) [mPa s]	582*	5347	4137
Pour point [°C]	15	27*	Nd
Max water content in lab [%]	67-81	19-50	49-70
Max water content in polludrome [%]	86	57	70

* from SINTEF

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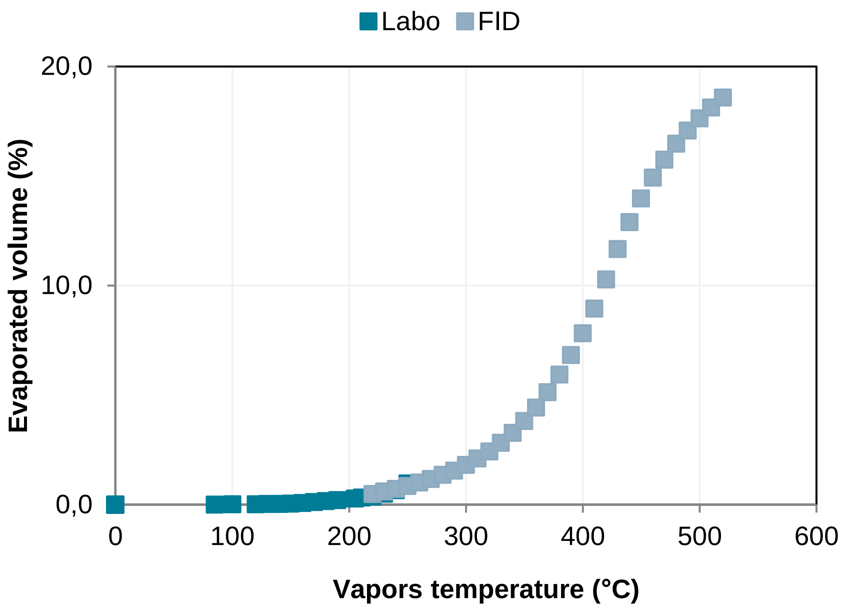
Lab characterization of the oil composition

Distillation curve



OSCAR characterization

Individuals compounds	Composition (% weight)
C_1-C_4 (dissolved gas)	0.03
C_5-saturates (n-/iso-/cyclo)	0.00
C_6- saturates (n-/iso-/cyclo)	0.00
C_7- saturates (n-/iso-/cyclo)	0.00
C_8- saturates (n-/iso-/cyclo)	0.00
C_9- saturates (n-/iso-/cyclo)	0.01
Benzene	0.00
C_1-Benzene	0.00
C_2-Benzenes	0.00
C_3-Benzenes	0.02
C_4 & C_5-Benzenes	0.00
C_{10}- saturates (n-/iso-/cyclo)	0.00
C_{11}-C_{12} (total saturates + aromatics)	4.01
C_{13}-C_{14} (total saturates + aromatics)	4.36
C_{15}-C_{16} (total saturates + aromatics)	4.47
C_{17}-C_{18} (total saturates + aromatics)	3.29
C_{19}-C_{20} (total saturates + aromatics)	3.33
C_{21}-C_{25} (total saturates + aromatics)	5.94
C_{25}+ (total)	71.66
Naphthalenes 1 (C_0-C_1 alkylated)	0.64
Naphthalenes 2 (C_2-C_3 alkylated)	0.40
PAHs 1 (medium solubility)	0.46
PAHs 2 (low solubility)	1.38
Phenols (C_0-C_4)	-

Each pseudo-component is characterized by density, molar mass, molar volume, vapour pressure, boiling point, solubility, photooxidation rate, biodegradation rate,...

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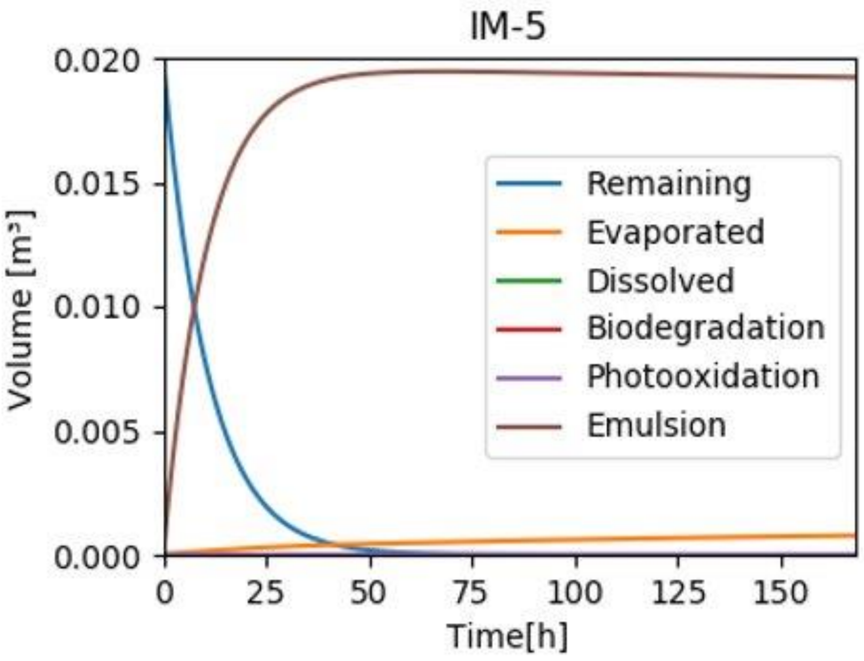
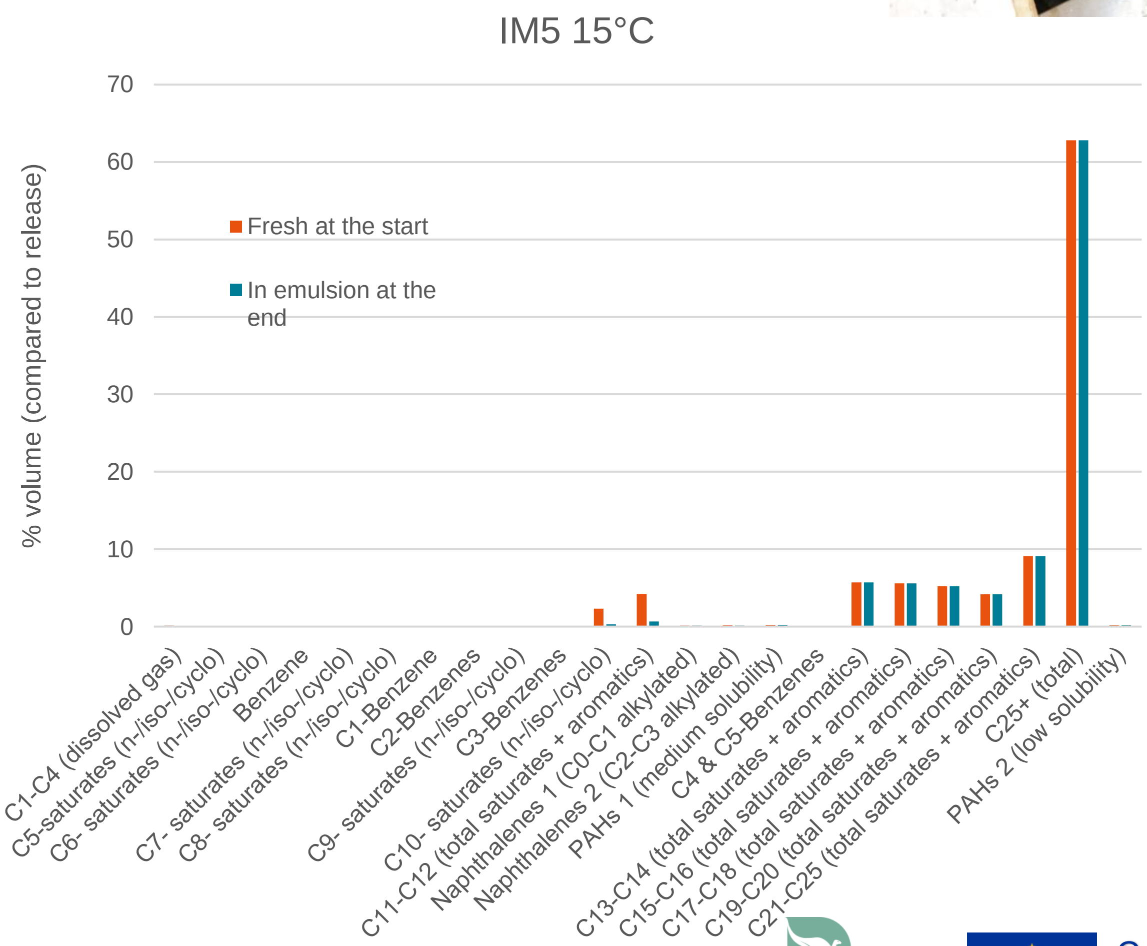
Model simulation IM-5 at 15°C





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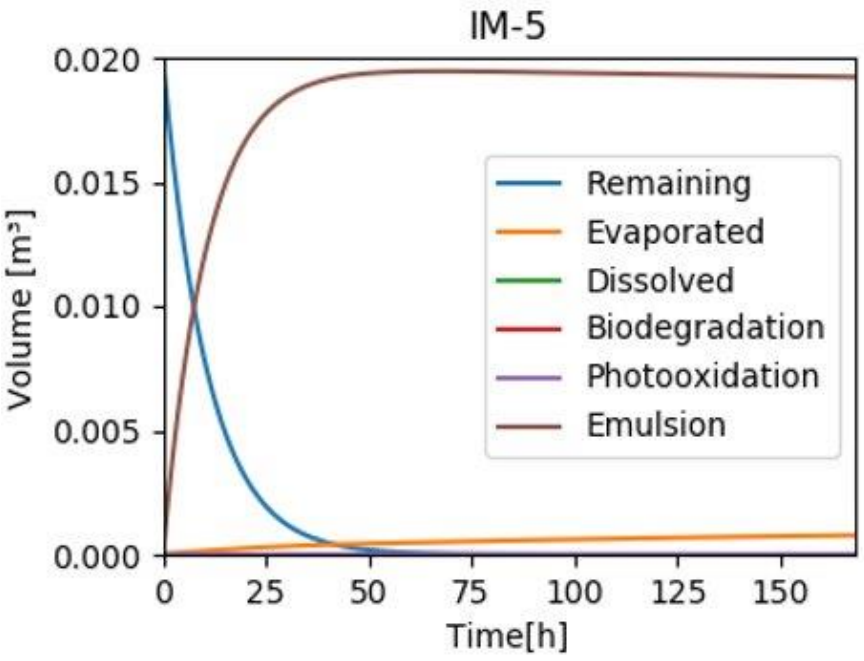
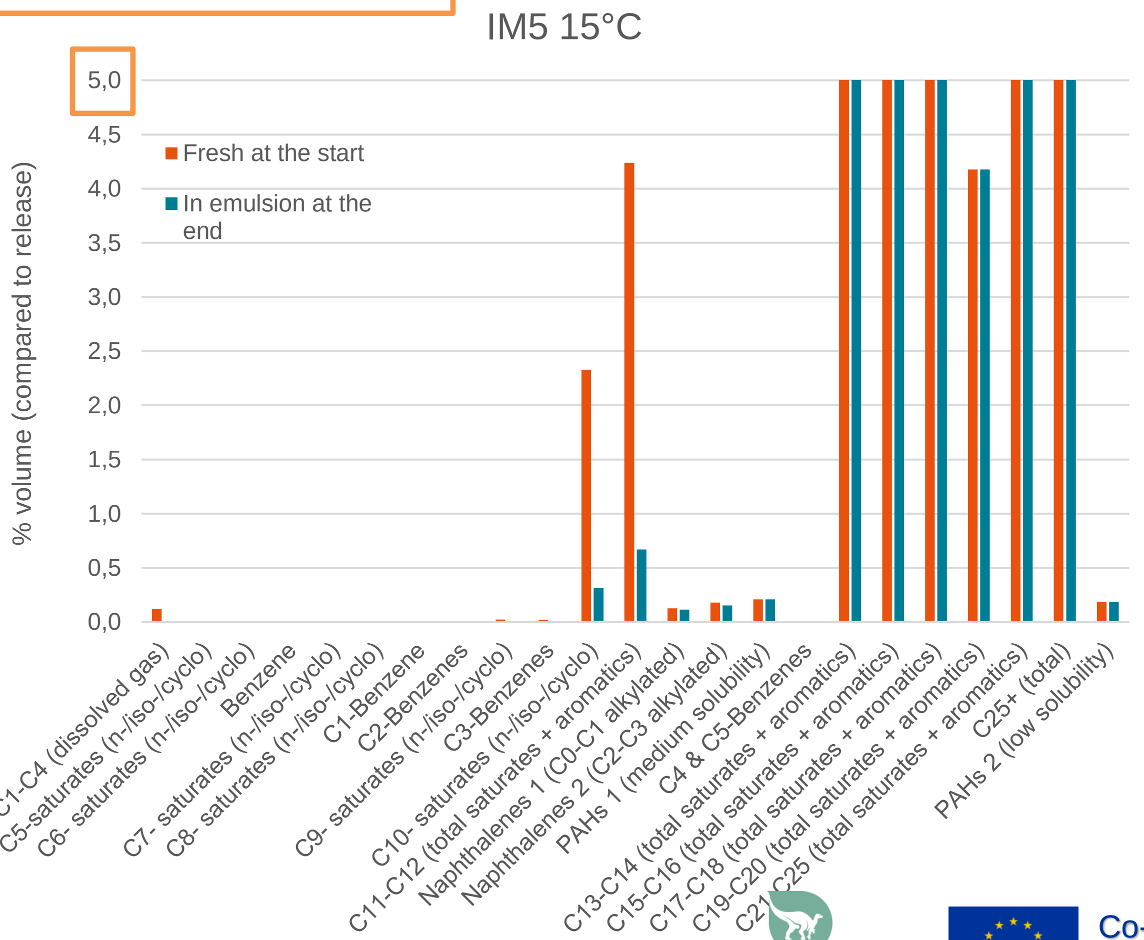
Model simulation IM-5 at 15°C

Zoom; C25+ = 62% volume





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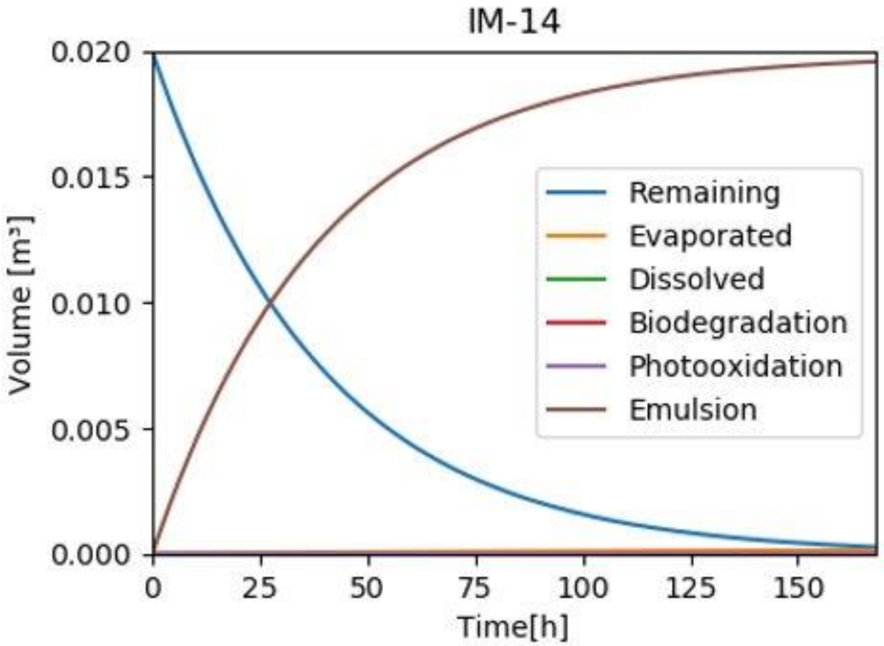
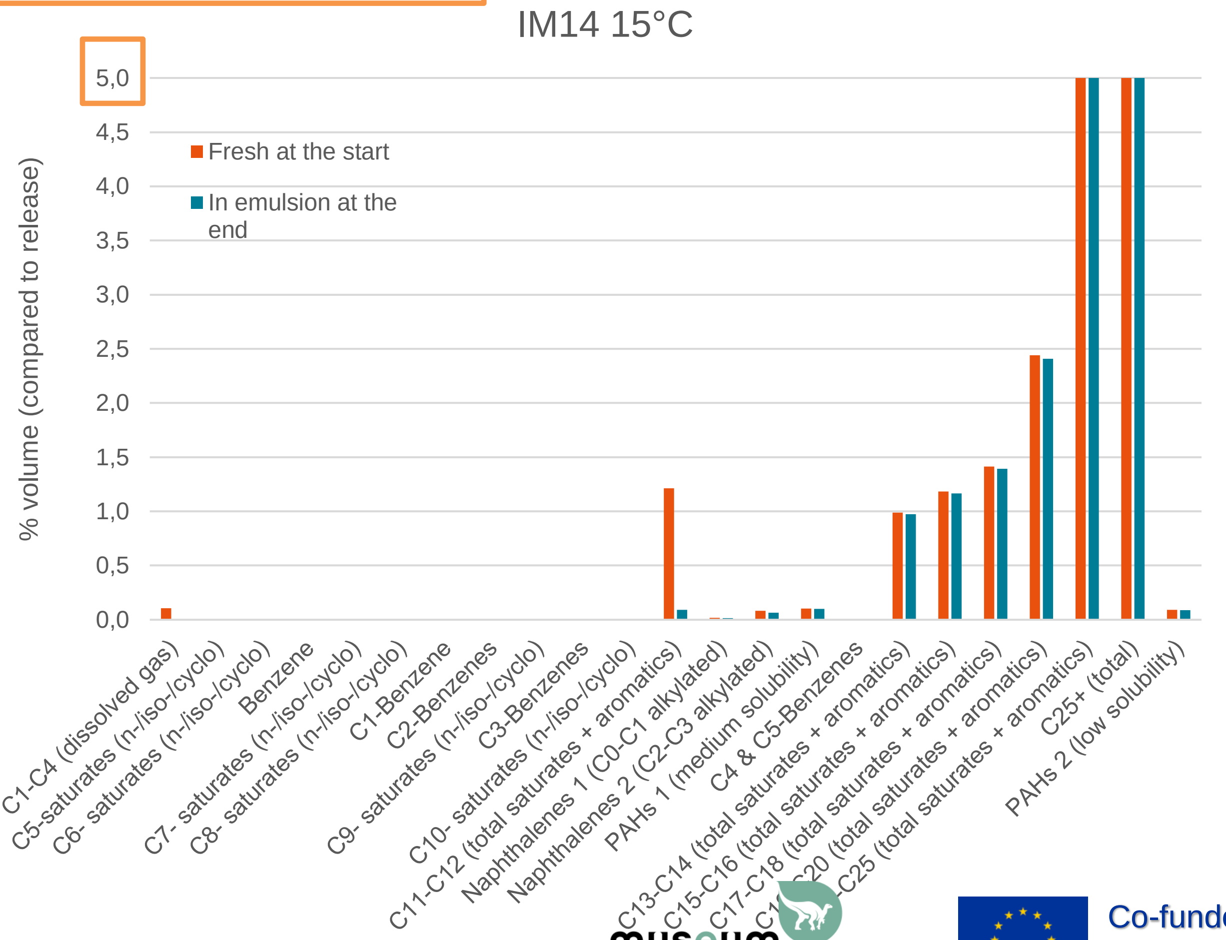
Model simulation IM-14 at 15°C

Zoom; C25+ = 81 % volume





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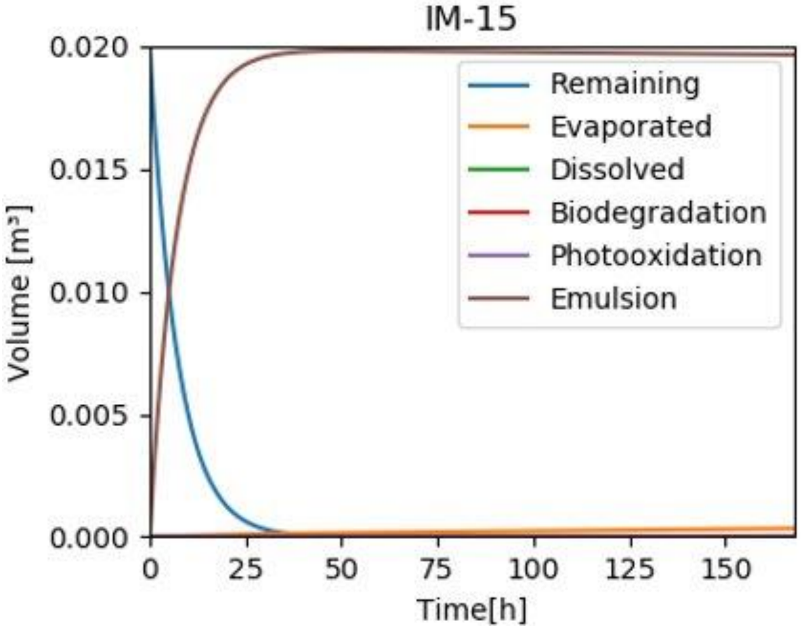
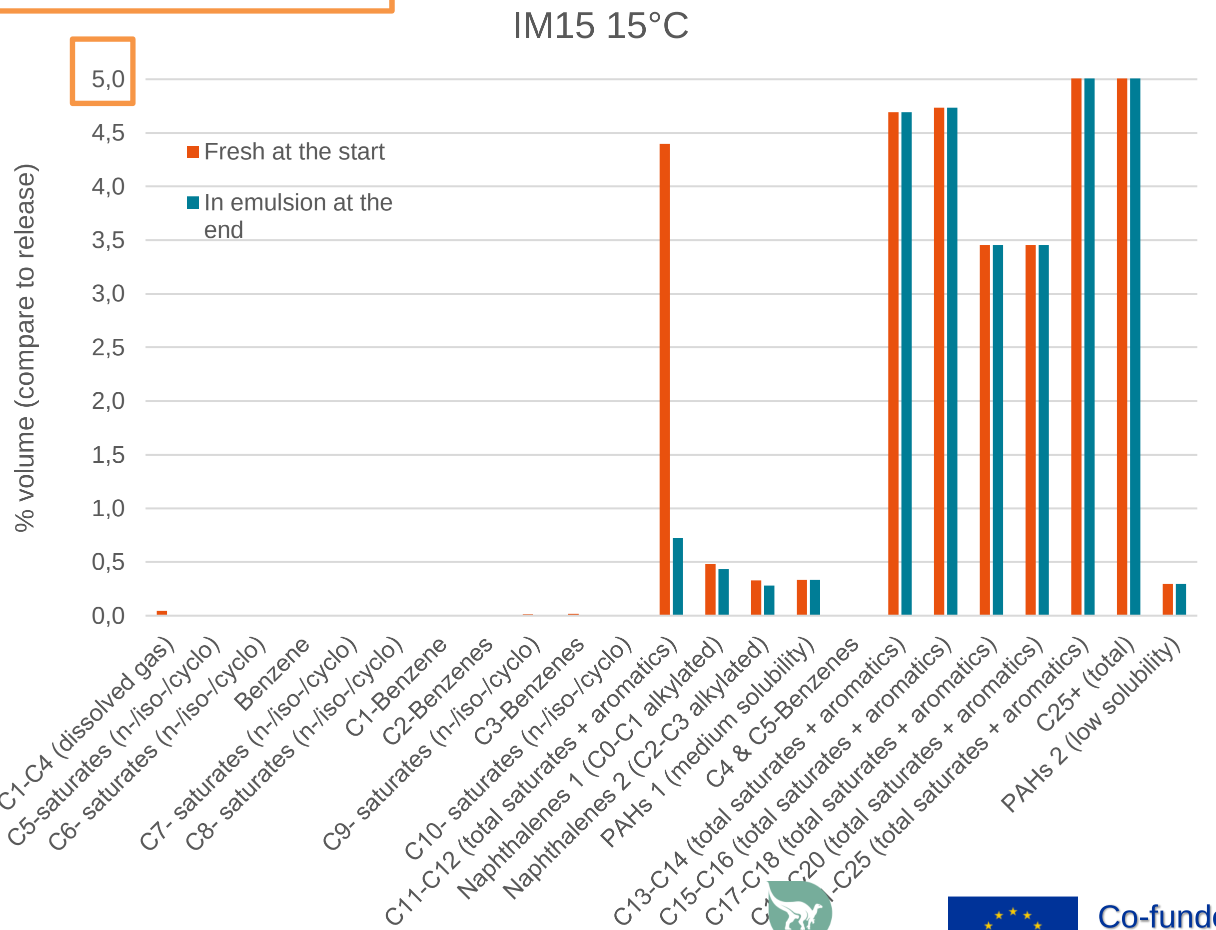
Model simulation IM-15 at 15°C

Zoom; C25+ = 71% volume





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Model simulations at 15°C

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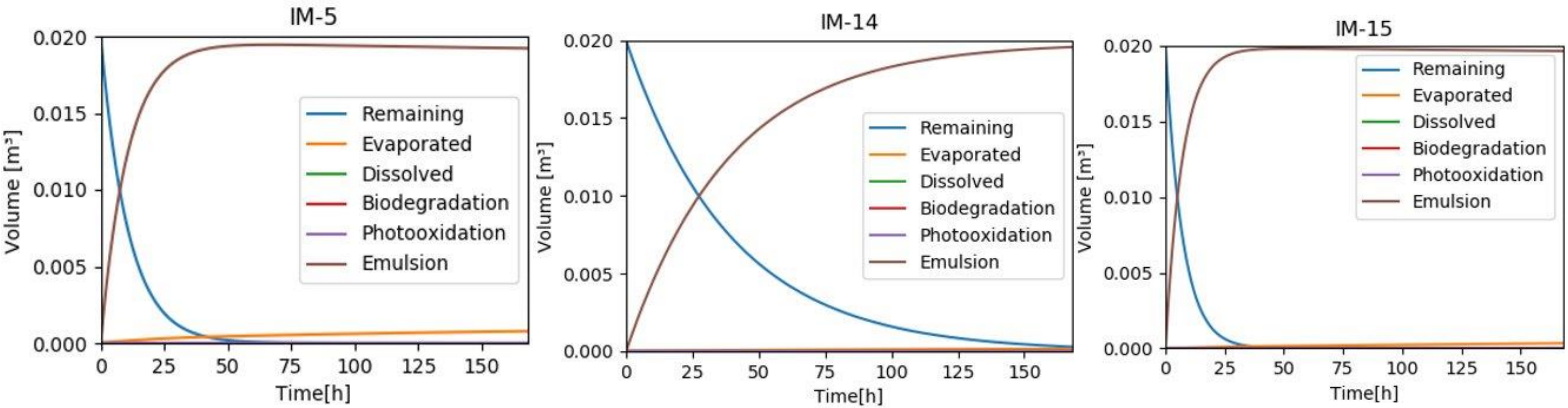

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Evaporation is slightly underestimated

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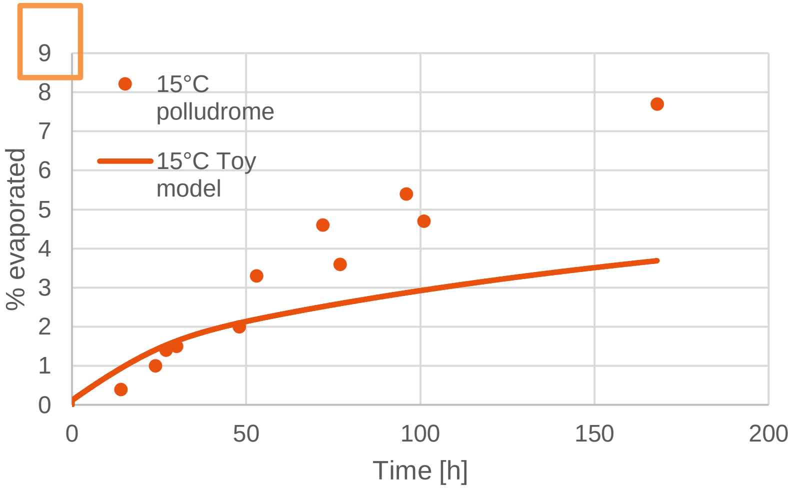
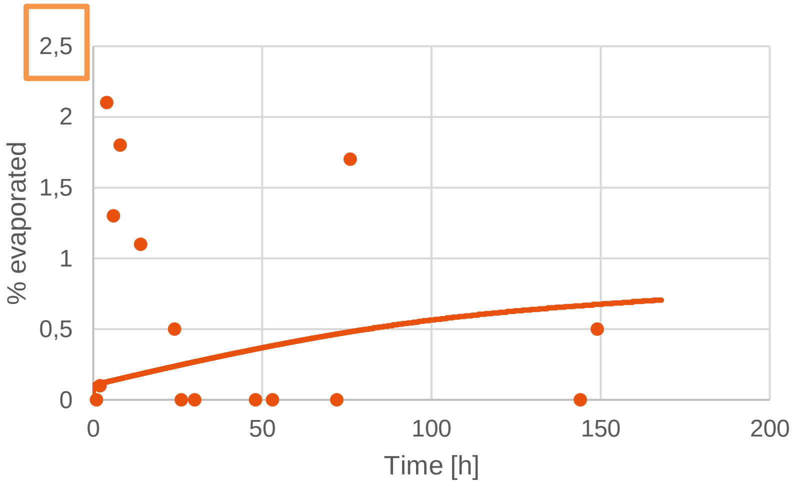
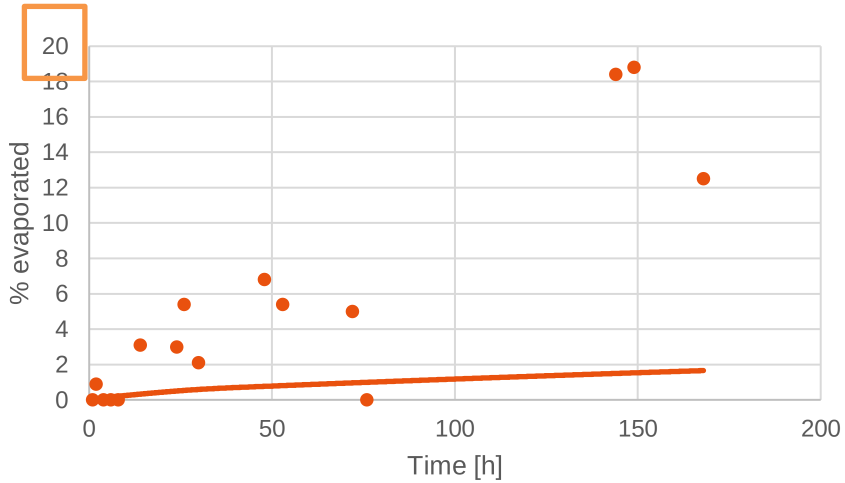
IM-5



IM-14



IM-15



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Evaporation is slightly underestimated

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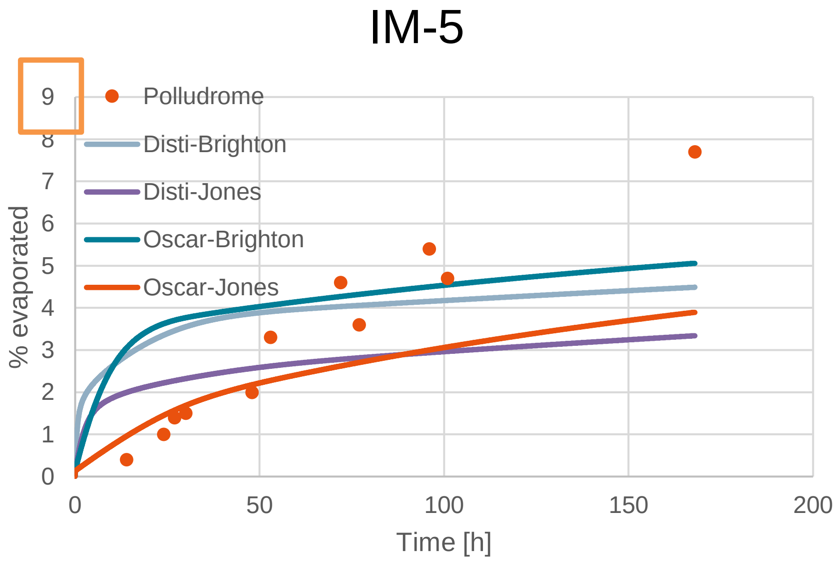

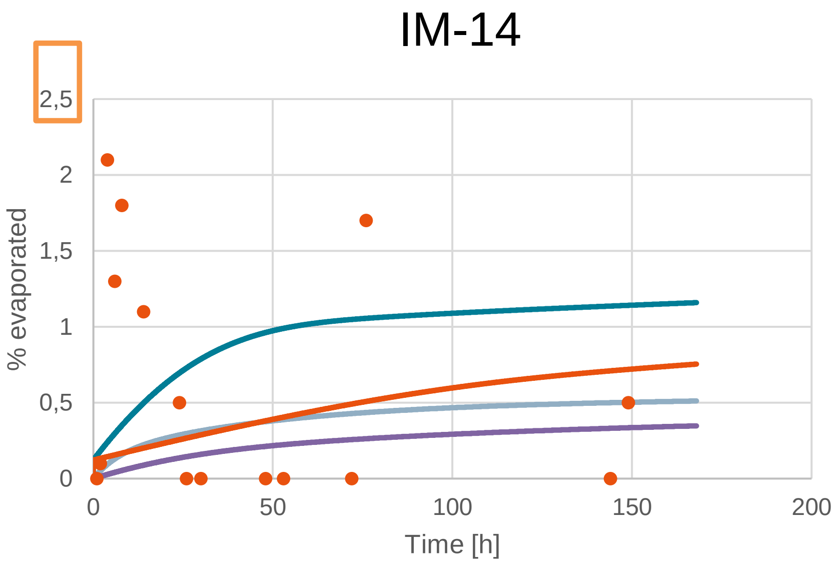

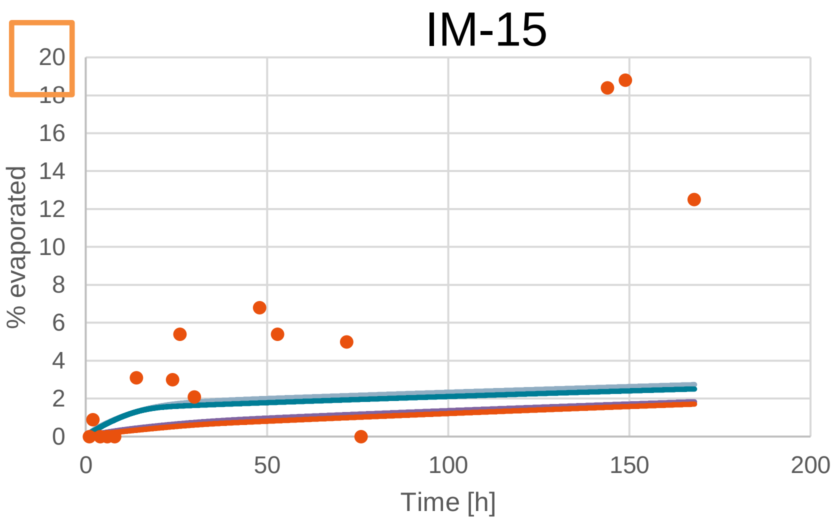

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Emulsion (Scory, 2005)

$$\frac{dV_{em}}{dt} = \frac{C_{18}}{1 - C_{18}} \frac{H_s}{C_{15}} V_r K_{em}$$

$$V_{water} = \frac{C_{18}}{1 - C_{18}} V_{em}$$

$$V_{tot,em} = V_{em} + V_{water} = \frac{1}{1 - C_{18}} V_{em}$$

$$V_{tot} = V_r + V_{em} + V_{water} = V_r + \frac{1}{1 - C_{18}} V_{em}$$

$$Y = \frac{V_{water}}{V_{tot}}$$

V_r : Volume of remaining oil [m³]
V_{em} : Volume of emulsified oil [m³]
V_{water}: Volume of water in the slick [m³]
$V_{tot,em}$: Total volume of the emulsion [m³]
V_{tot}: Total volume of the slick [m³]

Y : water fraction in the slick [%]

H_s : significant waves height [m]
C_{15} : scaling constant (2000000 m)
C_{18} : Maximum water content [%] (Lab)
K_{em} : kinetic coefficient (0-120) [s^{-1}]

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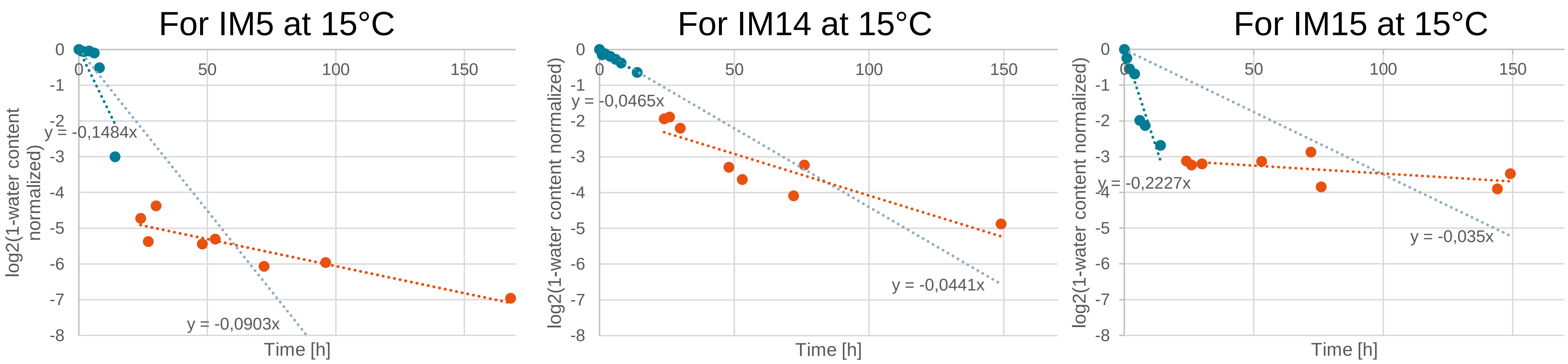
K_{em} can be estimated from water content evolution for the first 20h in polludrome



$$Kem = \left[t_{1/2} \frac{C_{18}}{1 - C_{18}} \frac{H_s}{C_{15}} \right]^{-1}$$

	IM-5	IM-14	IM-15
K_{em} [s^{-1}]	15,99	18,73	43,59

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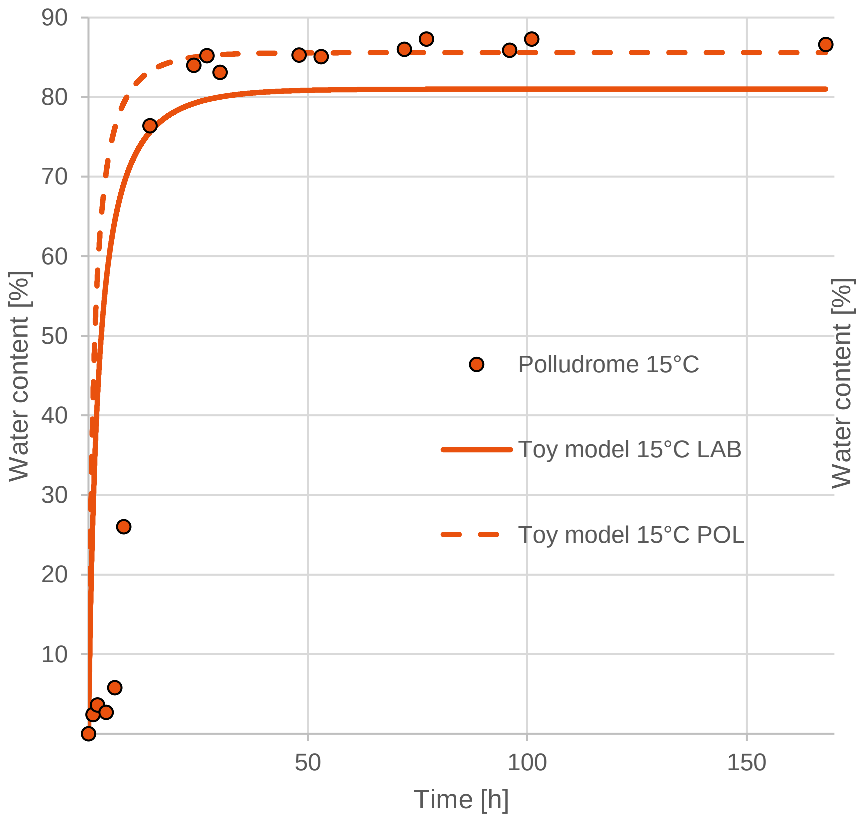
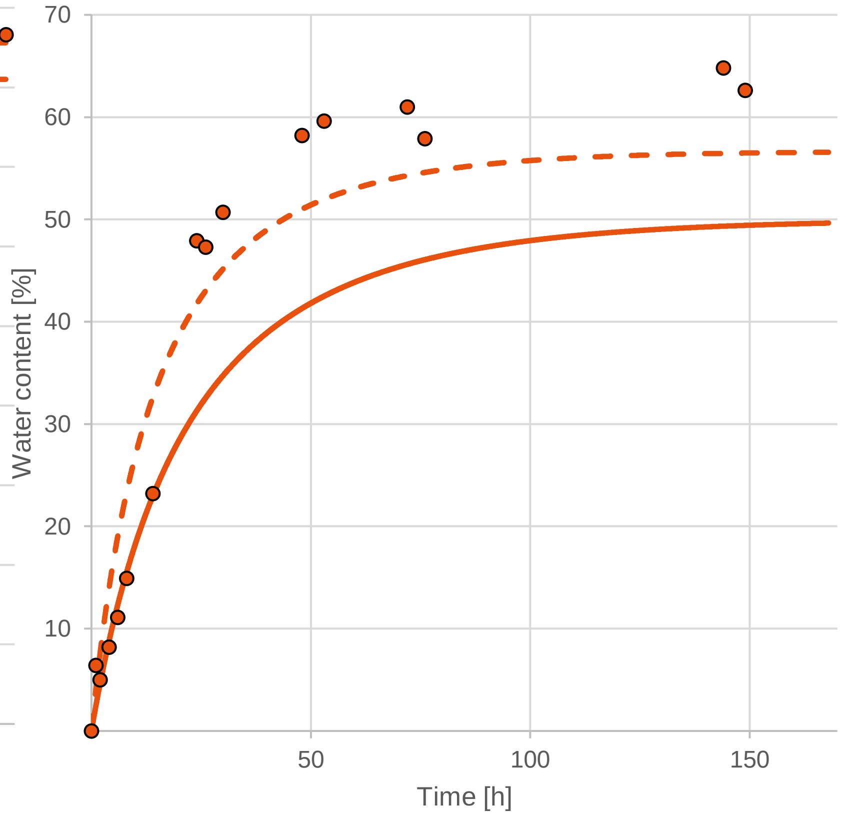
The Scory parametrization provides a good estimate of the water content [Y] uptake in the slick

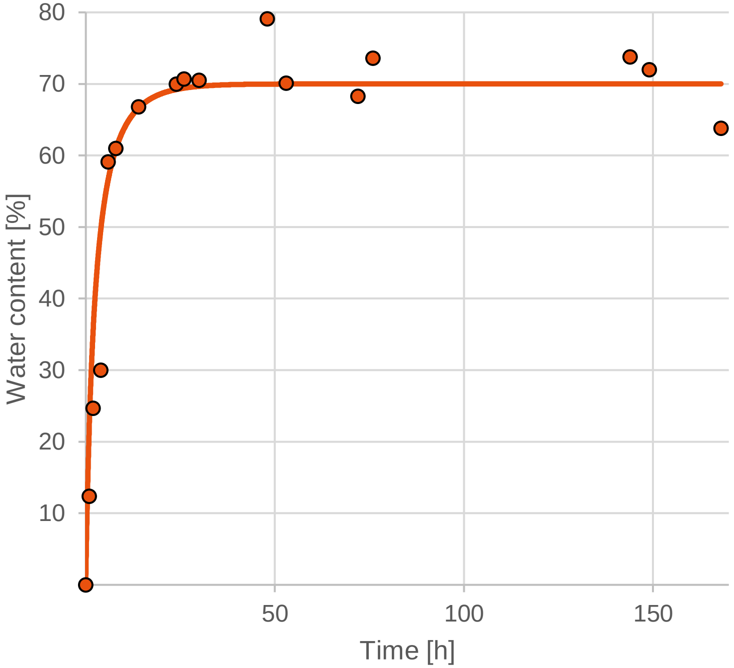
IM5



IM14



IM15



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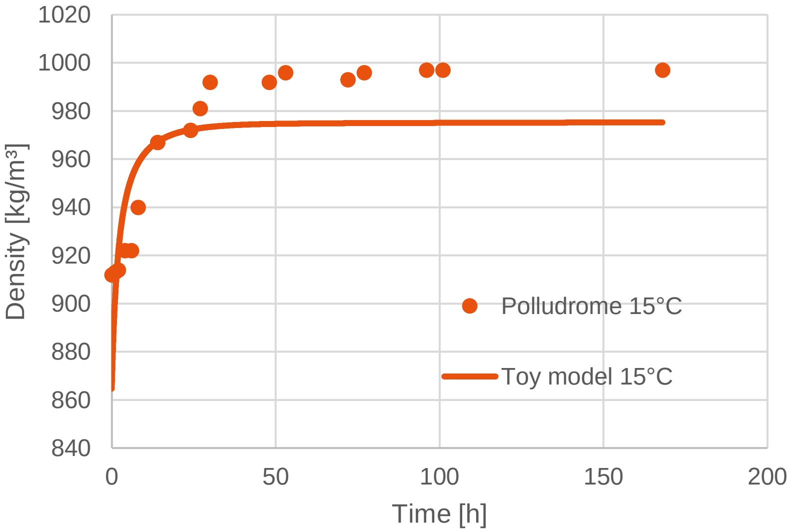
Model can simulate the evolution of the slick density if the fresh oil density is known

$$\rho_{C_{25}+} := \frac{\rho_{oil,fresh} V_{oil,init} - \sum \rho_i V_{i,init}}{V_{C_{25}+,init}}$$

$$\rho_{slick} = \frac{\sum \rho_i V_i + \rho_{water} V_{water}}{V_{tot}}$$

IM5



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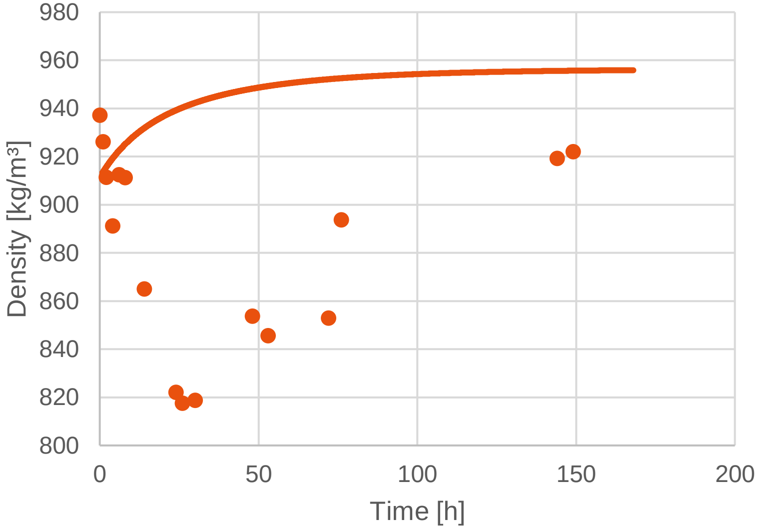

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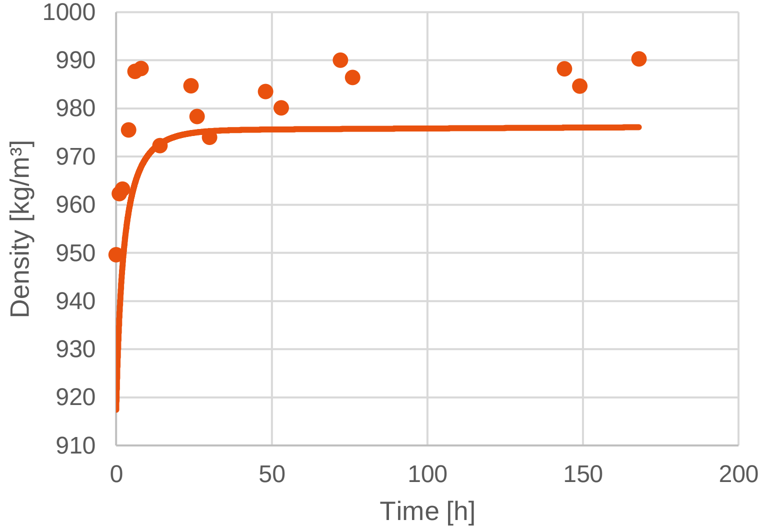

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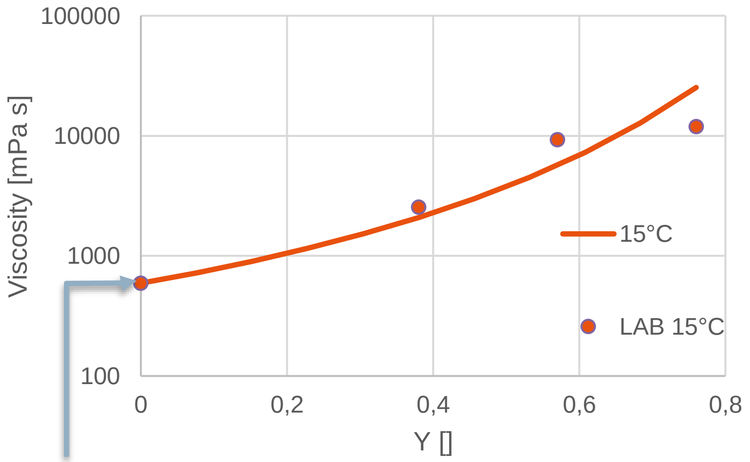
If non-emulsified oil viscosity is known, models can estimate viscosity of emulsified oil as a function of the water content

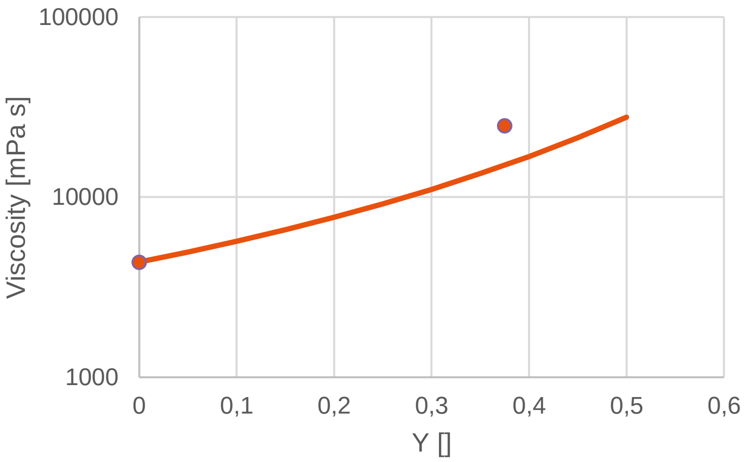
$$\upsilon_{oil} = \upsilon_{ref} \exp\left(\frac{C_{emul1} Y}{1 - C_{emul2} Y}\right)$$

(Betancour et al, 2005)

IM5



IM14



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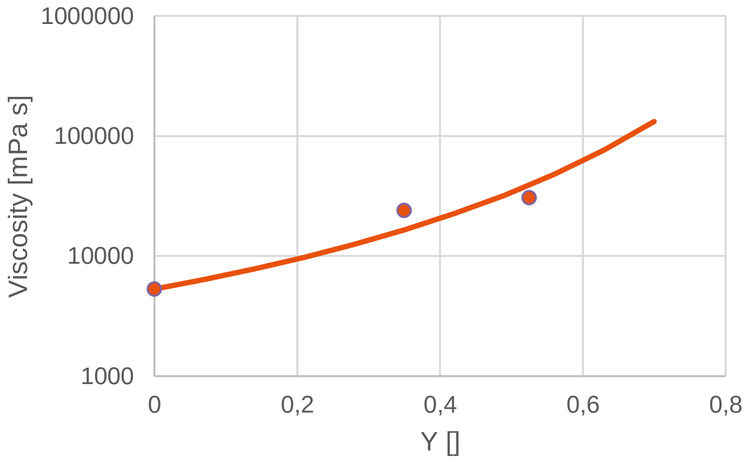

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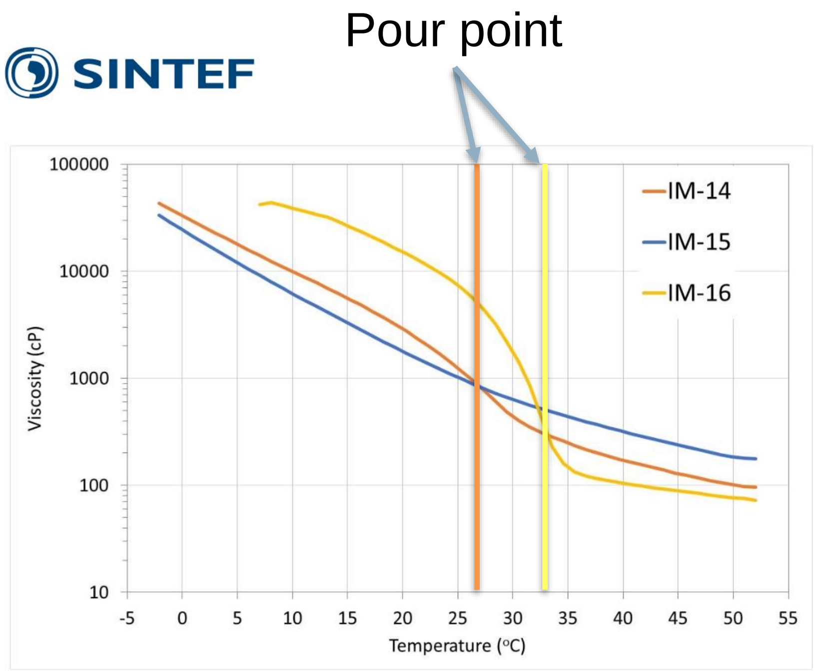
The viscosity of non emulsified oil depends on temperature and evaporation



$$\upsilon_{oil} = \upsilon_{ref} \exp\left(C_{temp} \left(\frac{1}{T} - \frac{1}{T_{ref}} \right) + C_{evap} F_{evap} \right)$$

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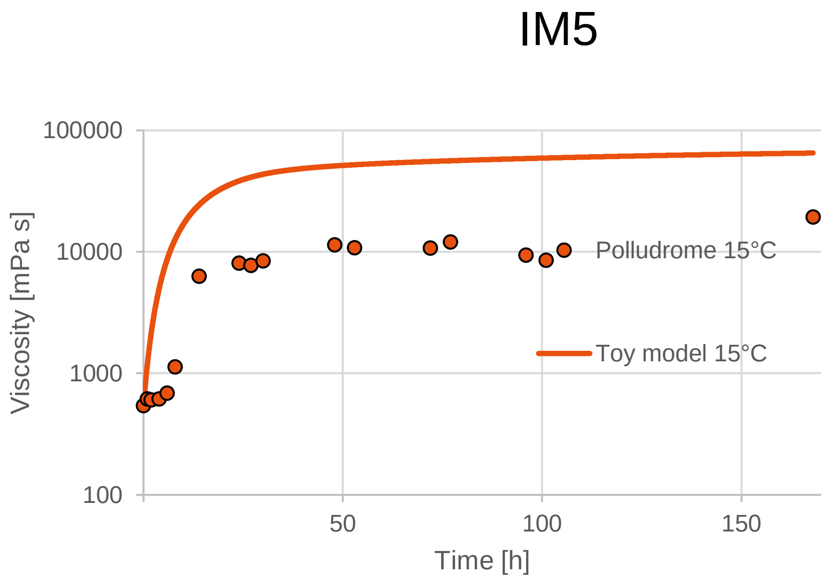
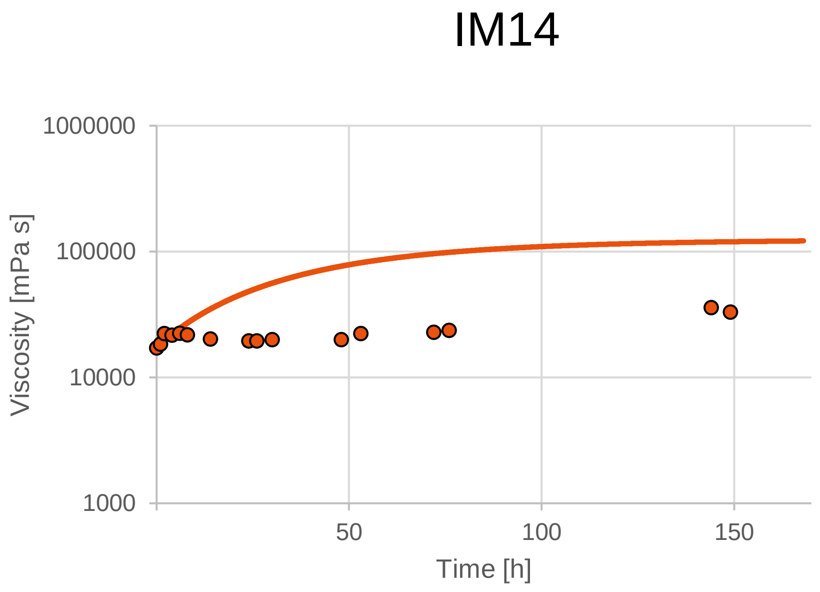
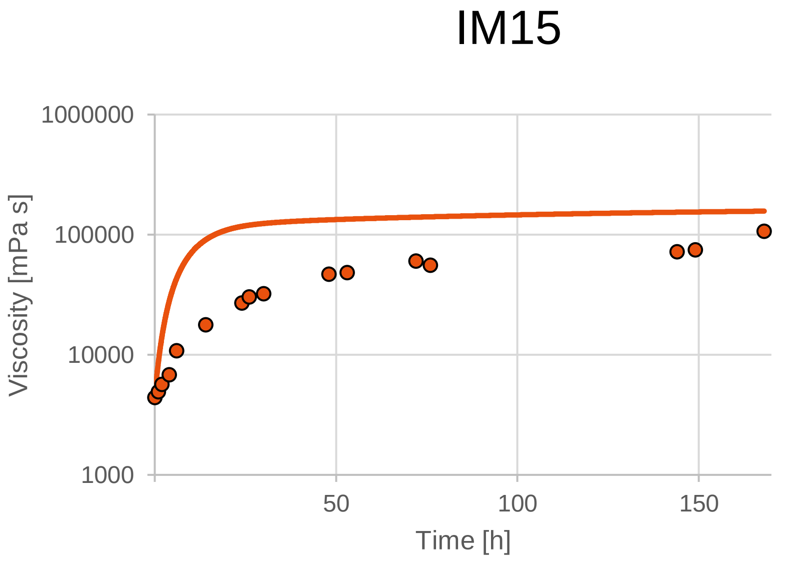
Model can make reasonable prediction of the evolution of slick viscosity

$$\upsilon_{oil} = \upsilon_{ref} \exp\left(C_{temp}\left(\frac{1}{T} - \frac{1}{T_{ref}}\right) + C_{evap}F_{evap} + \frac{C_{emul1}Y}{1 - C_{emul2}Y}\right)$$







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Take home message

Are the existing parameterizations able to simulate VLSFO weathering?

Yes, they can

Should you trust in oil weathering model forecast for VLSFO?

Only if an accurate oil characterization is available

Oil slick spreading should be improved to take into account the 'rheofluidity'

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