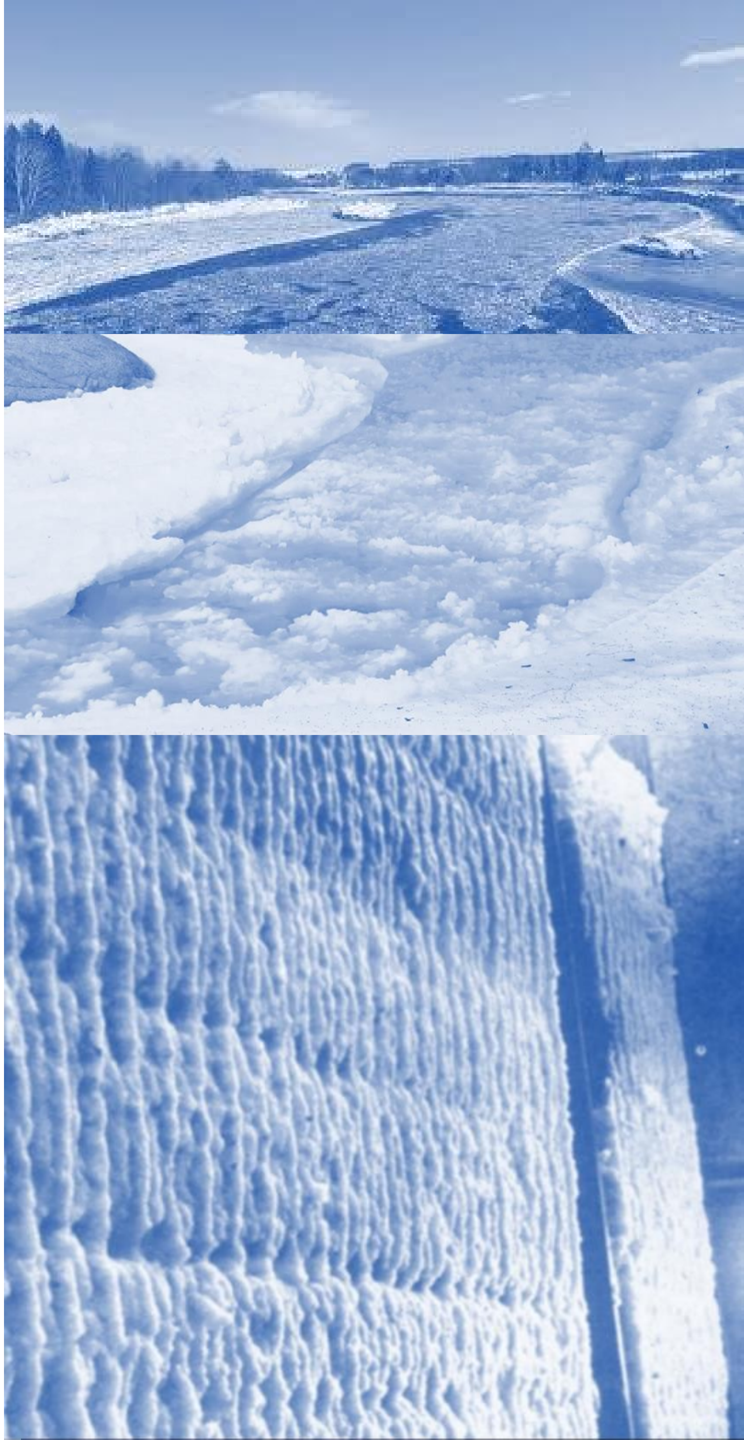
UNCERTAINTY ANALYSIS OF SINGLE- AND MULTIPLE-SIZE-CLASS **FRAZIL ICE MODELS**

Fabien SOUILLÉ, Cédric GOEURY, Rem-Sophia MOURADI,

“No one trusts a model except the man
who wrote it;
everyone trusts an observation, except the
man who made it.”
Harlow Shapely

23/06/2023

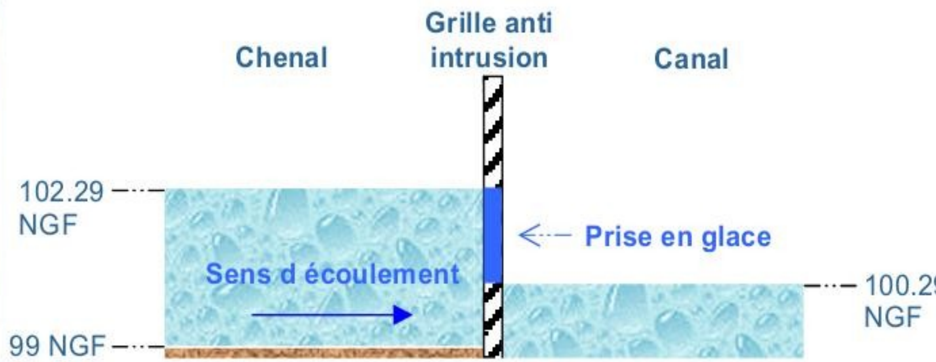


BACKGROUND AND OBJECTIVES

"Active" Frasil consists of ice particles suspended in supercooled water, which can adhere to submerged objects → can cause severe clogging of water intake trash racks

Historical events

- In **2008**, all NPP sites are considered at risk by default
- **January 9, 2009** → partial obstruction of the anti-intrusion grids of the **Chooz NPP**



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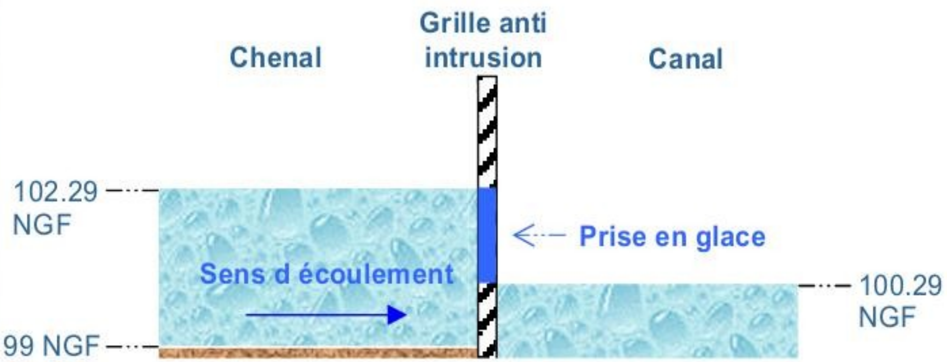
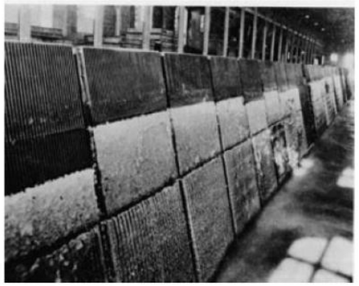


- Other clogging events (Canada / United States)

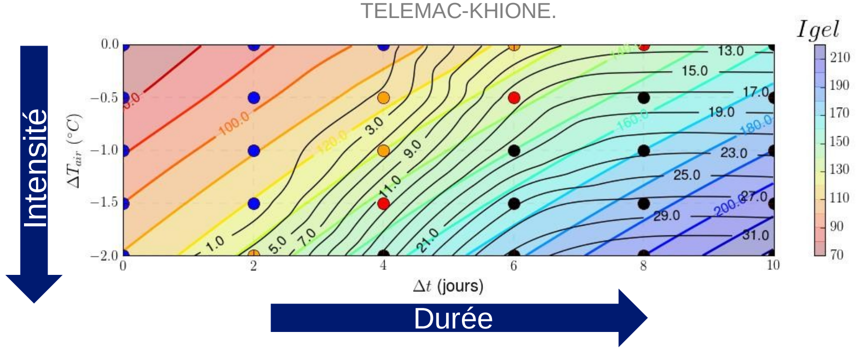


BACKGROUND AND OBJECTIVES

The LNHE and IGUASOU project :

- Water intake design and filtration system
- Frazil ice risk assessment
  - Characterization of the phenomenon
  - Assessment of the vulnerability of water intakes
  - Review of the sufficiency of existing mitigation

Example of clogging risk map obtained from numerical simulation using TELEMAC-KHIONE.



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Main tool : numerical modeling of free surface hydrodynamics

- **TELEMAC-MASCARET system**
- Shallow water equations solver (2D) and free surface Navier-Stokes equations (3D)
- Several modules are available to model various processes like the **KHIONE module for frazil ice**

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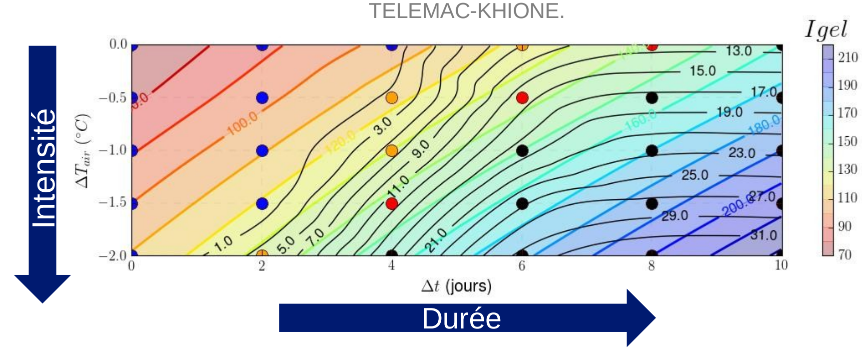
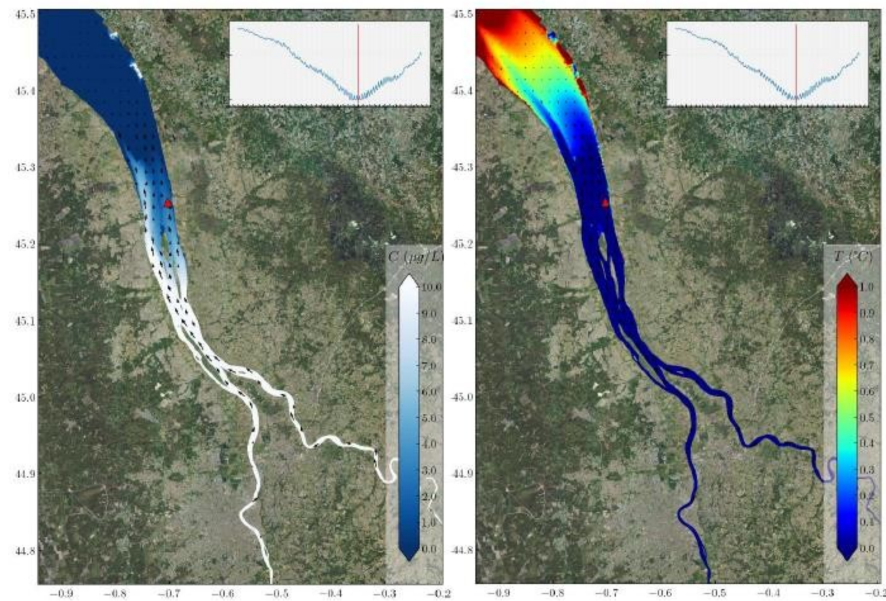




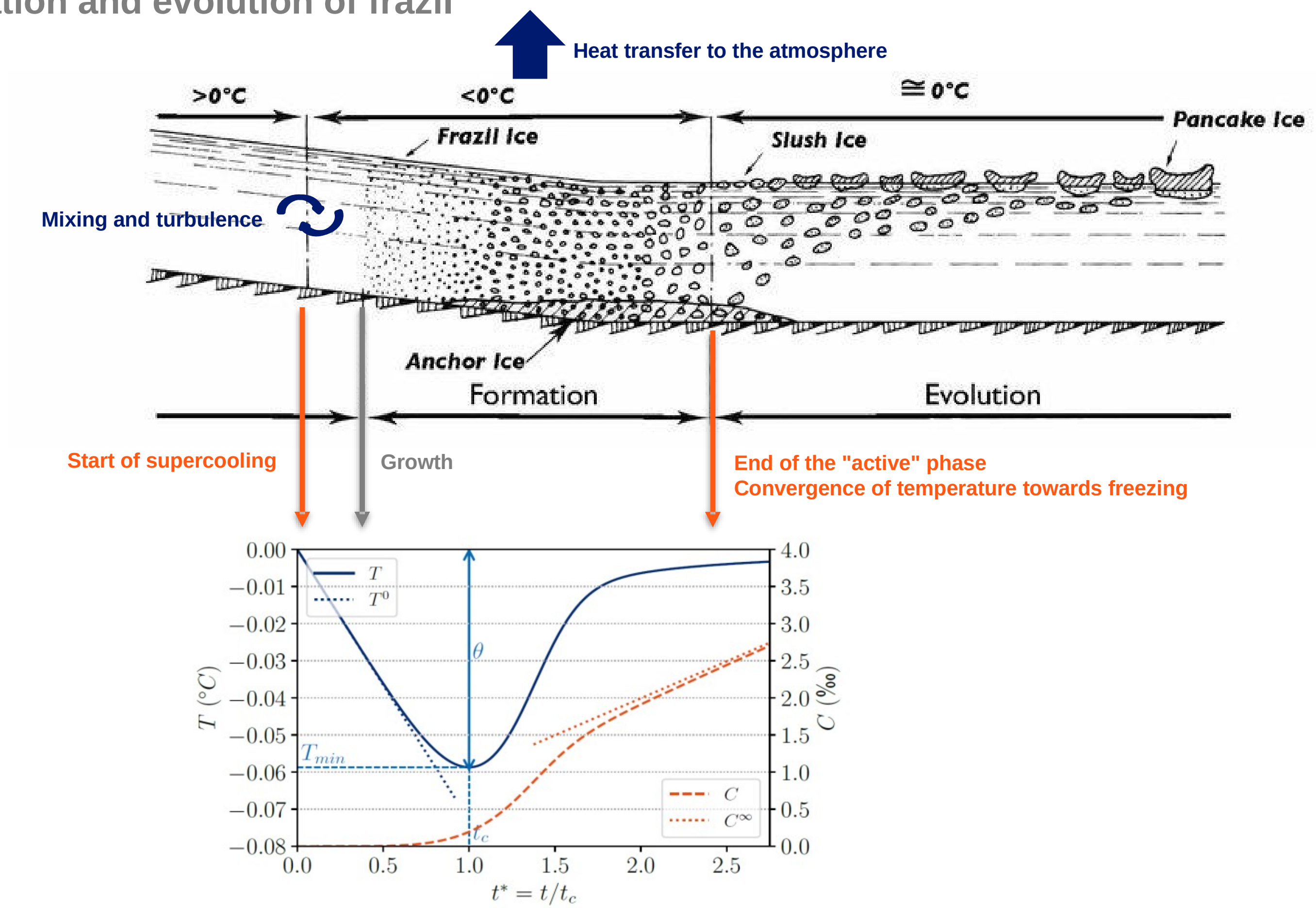
Example of numerical simulation of the Gironde estuary using TELEMAC-2D KHIONE during an extreme winter event. Frazil ice (left) and water temperature (right)

SOMMAIRE

SOMMAIRE

FRAZIL FORMATION AND SUPERCOOLING

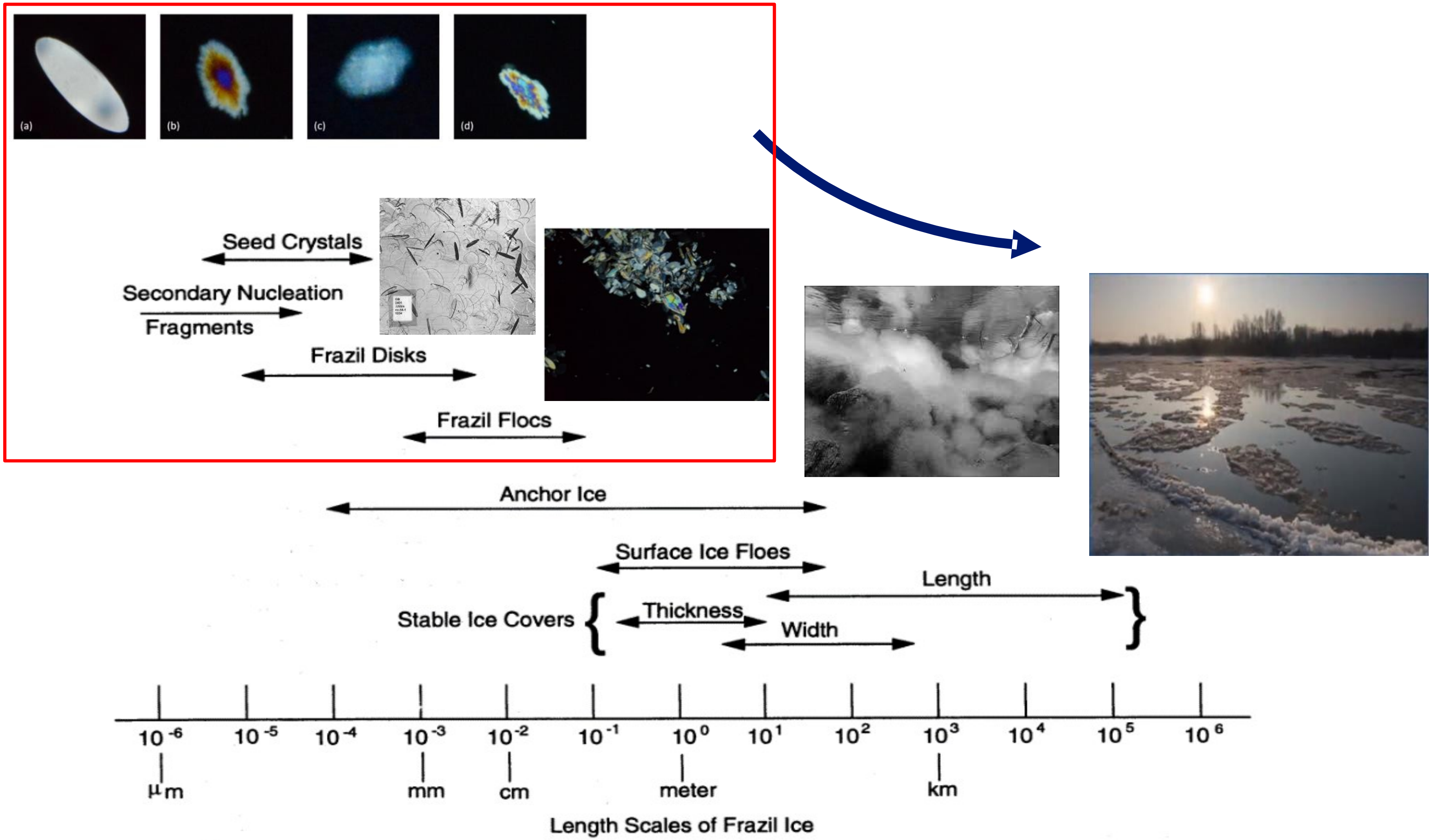
Formation and evolution of frazil



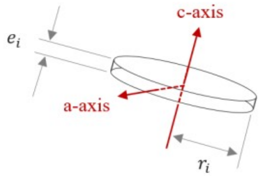
Water supercooling curve and evolution of the frazil volume fraction

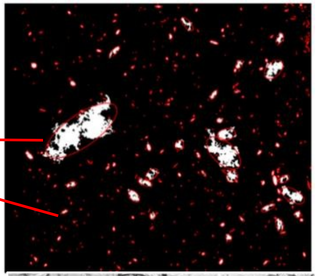
FORMS OF ICE IN RIVERS

Ice forms in rivers and scales



MODELLING ASSUMPTIONS





Shape of crystals and flocs: discs

- Radius: r
- Ratio between diameter and thickness assumed constant : $R = \frac{2r}{e}$

Fundamental equations of frazil dynamics (Daly 1984)

- Radial space : $\mathrm{n}(x, y, z, t, r)$ with $r \in [r_c, \infty[$
- PDE System

$$\frac{\partial n}{\partial t} + \mathbf{u}.\nabla n - \nabla.(\nu_c \nabla n) = -\underbrace{\frac{\partial}{\partial r}(Gn)}_{①} + \underbrace{\left(\dot{N}_T + \dot{N}_I\right)\delta(r - r_c)}_{②} - \underbrace{\frac{1}{V}\frac{\partial}{\partial r}(FVn)}_{③} - \underbrace{w_r\frac{\partial n}{\partial z}}_{④},$$

$$\frac{\partial T}{\partial t} + \mathbf{u}.\nabla T - \nabla.(\nu_t \nabla T) = \frac{\phi}{\rho c_p} + \frac{\rho_i L_i}{\rho c_p}\int_0^{\infty} Gandr,$$

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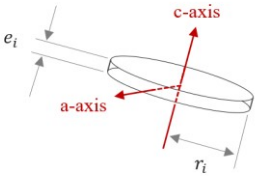

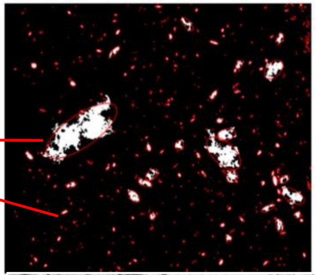

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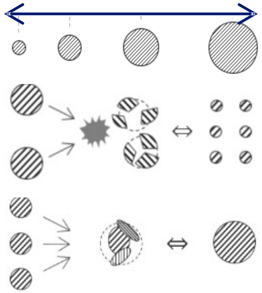
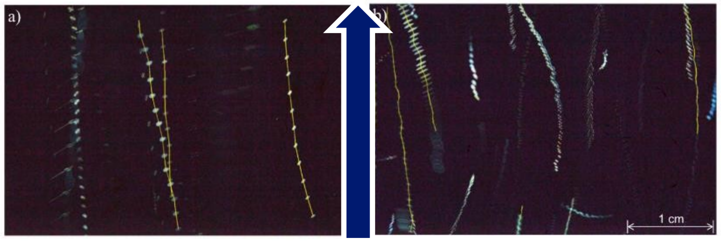
- Process
  1. **Thermal growth (G):** evolution of crystal size resulting from water change of state
  2. **Nucleation (N):** new primitive nuclei, by penetration at free surface or collisions
  3. **Flocculation (F):** agglomerate of particles resulting in large crystals
  4. **Buoyancy (wr):** particle and flocs rise to the surface (because of lower density)





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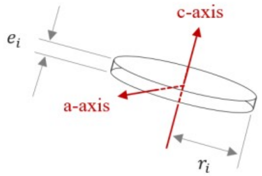

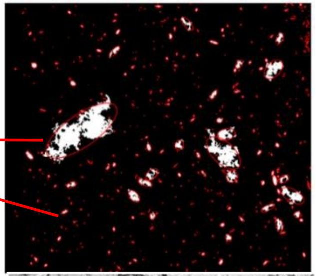

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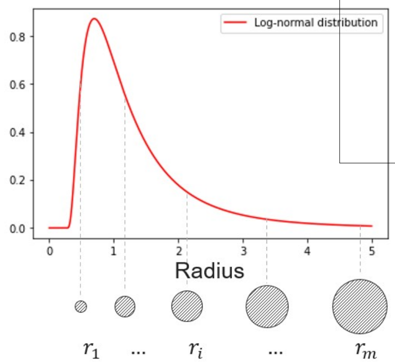
- How to solve the PDE system ?
  - **Spatial discretization:** for example TELEMAC (2D or 3D) or race-track hypothesis + well-mixed column (0D)
  - **Temporal discretization:** implicit pattern in time (very restrictive stability condition in explicit)
  - **Radial space discretization: MSC (Multiple-Size-Class) or SSC (Single-Size-Class simplification)**

MODELLING ASSUMPTIONS

Discretization of radial space

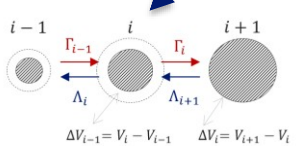
MSC (multiple-size-class) model

m Frazil volume fraction equations : c_i et $C = \sum_{i=1}^{m} c_i$
1 Temperature equation : T

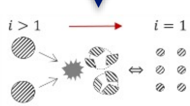


$$\frac{dT}{dt} = \frac{\phi}{\rho c_p} + \frac{\rho_i L_i}{\rho c_p} \sum_{i=1}^{m} S_i,$$

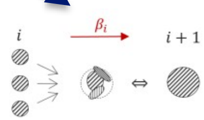
$$\frac{dc_i}{dt} = \underbrace{V_i\left(\Gamma_{i-1}c_{i-1} + (\Lambda_i - \Gamma_i)c_i - \Lambda_{i+1}c_{i+1}\right)}_{S_i,\ ①} + \underbrace{\tau_i}_{②} + \underbrace{\beta_{i-1}c_{i-1} - \beta_i c_i}_{③} - \underbrace{\gamma_i c_i}_{④} \quad (1 \leq i \leq m),$$



Thermal growth



Nucleation

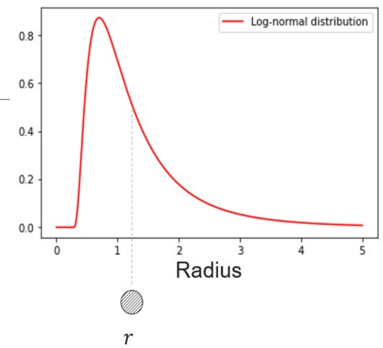


Flocculation

Simplification

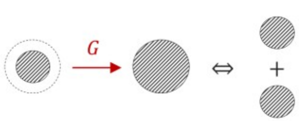
SSC (single-size-class) model

1 Frazil volume fraction equation : C
1 Temperature equation : T



$$\frac{dT}{dt} = \frac{\phi}{\rho c_p} + \frac{\rho_i L_i}{\rho c_p} GaN,$$

$$\frac{dC}{dt} = GaN + \frac{1}{h}\left(V\tau_s - w_r a_d C\right),$$



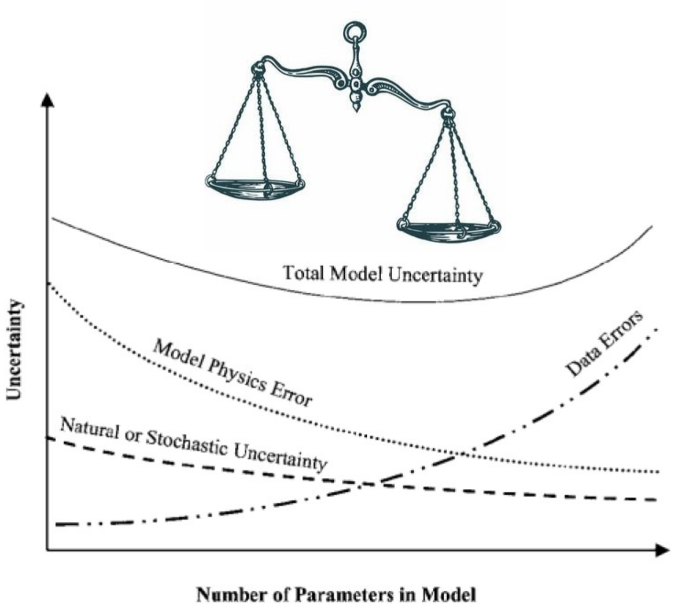
Thermal growth

OBJECTIVE OF THE UNCERTAINTY ANALYSIS

Complex physical phenomena : multiple scales & interactions
Can we trust numerical models ?
Model complexity versus uncertainty ?

Objectives the uncertainty analysis using OpenTURNS

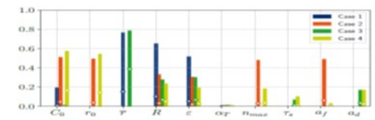
- Provide quantitative insight into the relative importance of contributing uncertain parameters,
- Help identify parameters for optimal calibration,
- Compare the output scatter of frazil ice models with single and multiple crystal size classes.



SOMMAIRE ✦

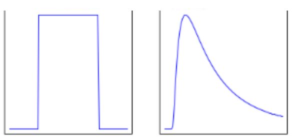
BASIC STEPS OF THE STUDY

Step C'
Hierarchy of parameters



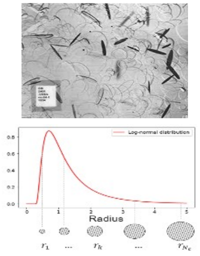
Step B
Uncertainty quantification

Modeling input distributions



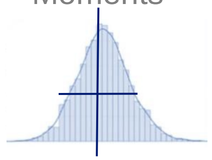
Step A
Problem specification

- Real system
- Input variables
- Numerical model
- Output variables



Step C
Uncertainty Propagation

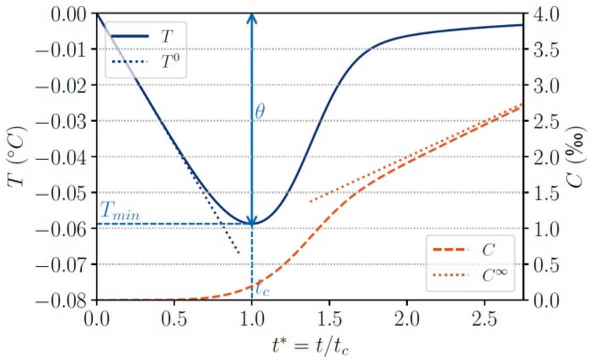
Quantities of interest : Moments



A – SPECIFICATION OF THE PROBLEM

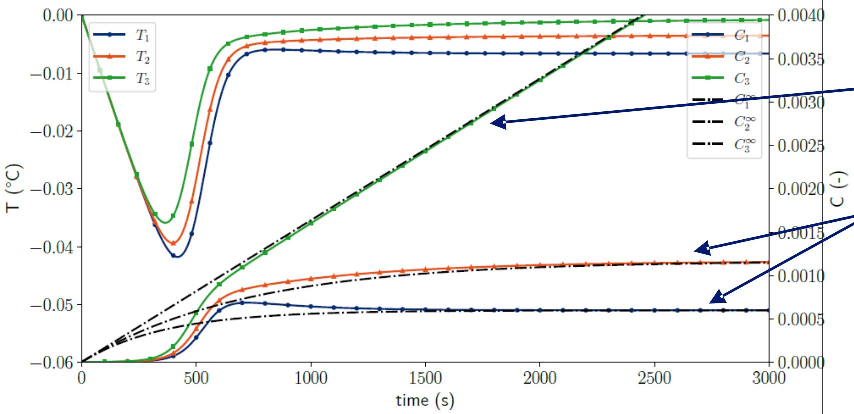
Supercooling of a “well mixed” volume of water

- Well-mixed volume hypothesis: $n(x, y, z, t, r) \sim n(t, r)$
- Heat loss to the atmosphere ϕ (W$/m^3$) assumed constant
- Focus on the transient phase (maximum supercooling) + steady state
- Output variables: $\boldsymbol{T(t), C(t) = g(X, d)}$
- Frasil models g : **SSC** (Single-Size-Class) or **MSC** (Multiple-Size-Class)
- Numerical resolution of semi-implicit EDO systems with dt=0.25s and convergence for the MSC model ($m = 100$)



Study of two cases (steady state ≠)

- **Without flotation:** linear divergence of frazil concentration
- **With flotation:** convergence towards an equilibrium concentration



$$C^\infty = C_0 - \phi t/\rho_i L_i.$$

$$C^\infty = \frac{h}{a_d w_r}\left(-\frac{\phi}{\rho_i L_i} + \frac{V\tau_s}{h}\right).$$

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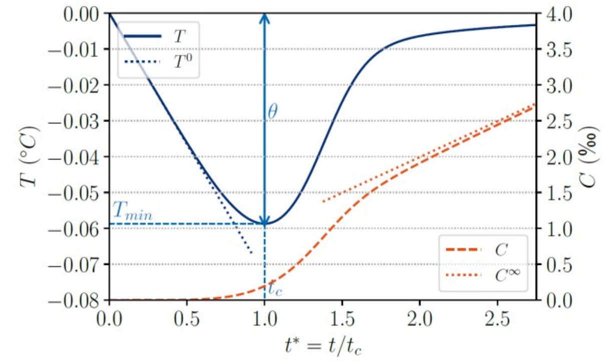


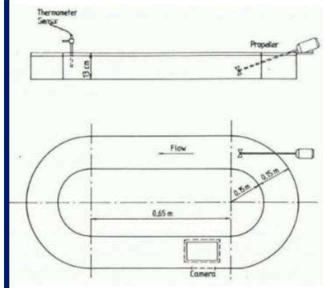
List of uncertain parameters (X)

Parameter	Unit	Description	Category	Model
C_0	-	Initial frazil volume fraction	Initial condition	Both
r_0	m	Initial maximum radius	Initial condition	MSC
r_{min}	m	Minimum radius	Discretization	MSC
r_{max}	m	Maximum radius	Discretization	MSC
$\overline{r}$	m	Mean radius	Discretization	SSC
R	-	Diameter to thickness ratio	Source term ①	Both
δ_T	m	Thermal growth length scale	Source term ①	Both
ε	$m^2.s^{-3}$	Turbulent dissipation rate	Source terms ①, ②	Both
α_T	-	Turbulent intensity	Source term ①	Both
n_{max}	m^{-3}	Secondary nucleation efficiency cap	Source term ②	MSC
τ_s	$m^{-2}.s^{-1}$	Seeding rate	Source term ②	Both
a_f	s^{-1}	Flocculation coefficient	Source term ③	MSC
a_d	-	Buoyancy coefficient	Source term ④	Both

TABLE 1 – Description of uncertain parameters of the frazil ice models.

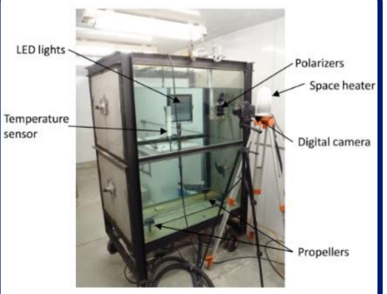
B – UNCERTAINTY QUANTIFICATION

Examples of experimental setup

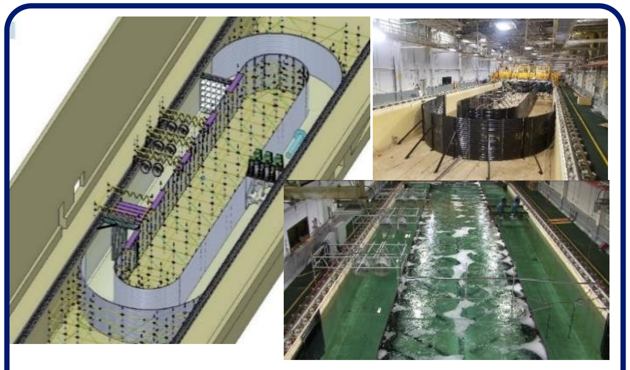


Carstens (1966)
Tsang & Hanley (1985)

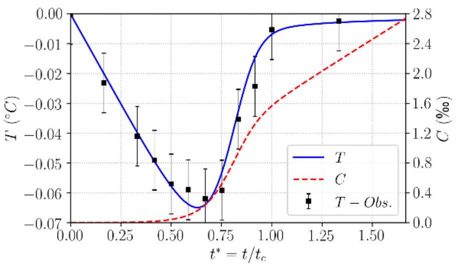
Clark & Doering (2006)



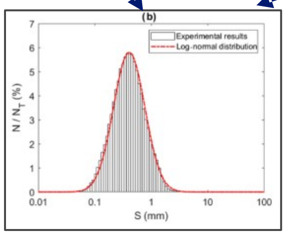
Schneck & al. (2019)



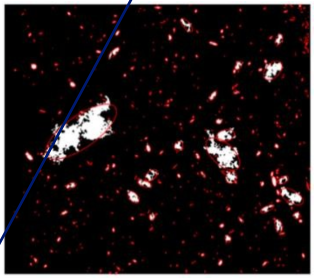
Projet EDF R&D / CNRC (2022)

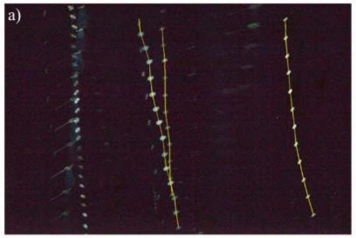


Supercooling curves (temperature)

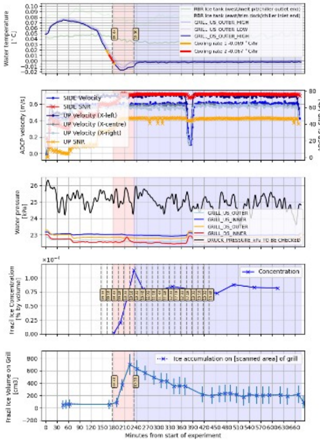


Frazil size distribution

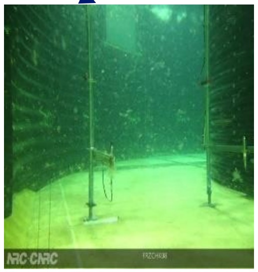


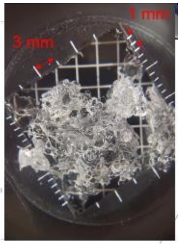


Frazil rise velocity



Complete chain of measurements from supercooling to clogging of grids

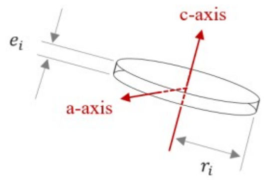




B – UNCERTAINTY QUANTIFICATION

Uncertain parameters

- Geometric properties of crystals
- Initial system condition
- Thermal growth and turbulence
- Nucleation / Flocculation
- Buoyant rise speed



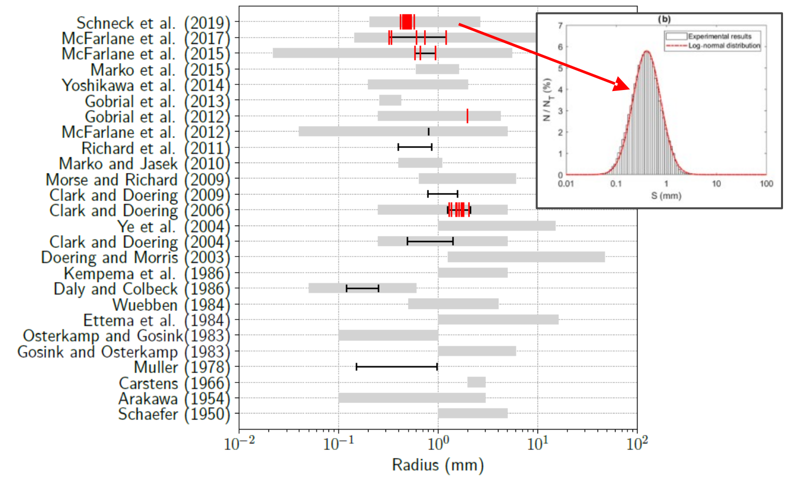


FIGURE 3 – Particle size ranges (thick grey line), mean range (thin dark line) and log-normal distributions' mean radius (red vertical ticks) reported in field or laboratory experiments (Schaefer, 1950, Arakawa, 1954, Carstens, 1966, Gosink and Osterkamp, 1983, Osterkamp and Gosink, 1983a, Ettema et al., 1984, Wuebben, 1984, Kempema et al., 1986, Daly and Colbeck, 1986, Doering and Morris, 2003, Ye et al., 2004, Ye and Doering, 2004, Clark and Doering, 2004, 2006, 2009, Marko and Jasek, 2010, Ghobrial et al., 2012, McFarlane et al., 2012, Ghobrial et al., 2013, McFarlane et al., 2015, Kempema and Ettema, 2016, McFarlane et al., 2016, 2017, Schneck et al., 2019)

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- Initial system condition
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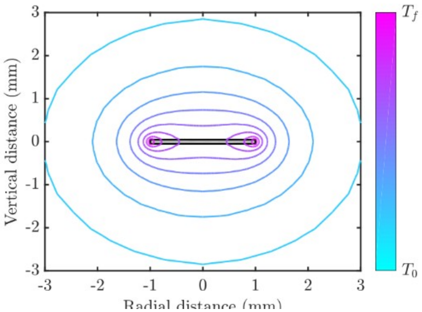
- Nucleation / Flocculation
- Buoyant rise speed

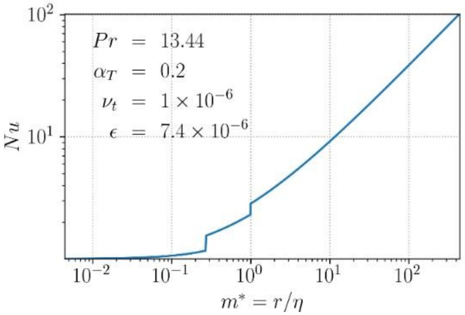
Radial growth rate — Nusselt number

$$\rho_i L_i G = \frac{N u k_w}{\delta_T} \Delta T,$$

Latent heat of freezing — Supercooling level

Thermal boundary layer thickness





$$Nu = \begin{cases} 1 + 0.17 m^* P_r^{1/2} & \text{if} \quad m^* \leq P_r^{-1/2} \\ 1 + 0.55 m^{*2/3} P_r^{1/3} & \text{if} \quad P_r^{-1/2} < m^* \leq 1, \end{cases}$$

$$Nu = \begin{cases} 1.1 + 0.77 \alpha_T^{0.035} m^{*2/3} P_r^{1/3} & \text{if} \quad \alpha_T {m^*}^{4/3} \leq 1000 \\ 1.1 + 0.77 \alpha_T^{0.25} m^* P_r^{1/3} & \text{if} \quad \alpha_T {m^*}^{4/3} > 1000, \end{cases}$$

B – UNCERTAINTY QUANTIFICATION

Uncertain parameters

- Geometric properties of crystals
- Initial system condition
- Thermal growth and turbulence
- Nucleation / Flocculation
- Buoyant rise speed

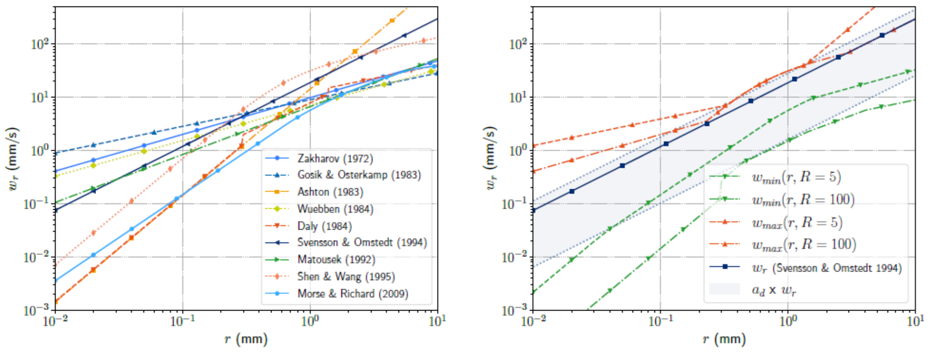


FIGURE 4 – Comparison of frazil rise velocity models with $R = 10$ (left) and rise velocity envelope chosen for the uncertainty analysis (right) (Zacharov et al., 1972, Gosink and Osterkamp, 1983, Ashton, 1983, Wueben, 1984, Daly, 1984, Svensson and Omstedt, 1994, Matoušek, 1992, Shen and Wang, 1995, Morse and Richard, 2009)

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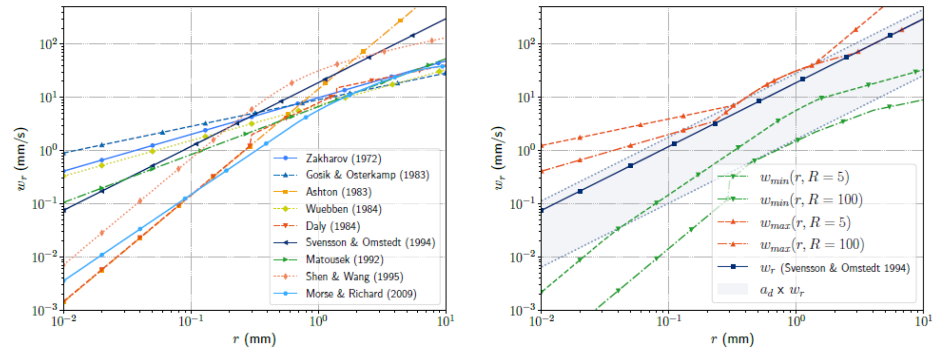


FIGURE 4 – Comparison of frazil rise velocity models with $R = 10$ (left) and rise velocity envelope chosen for the uncertainty analysis (right) (Zacharov et al., 1972, Gosink and Osterkamp, 1983, Ashton, 1983, Wueben, 1984, Daly, 1984, Svensson and Omstedt, 1994, Matoušek, 1992, Shen and Wang, 1995, Morse and Richard, 2009)

Summary of uncertain parameters

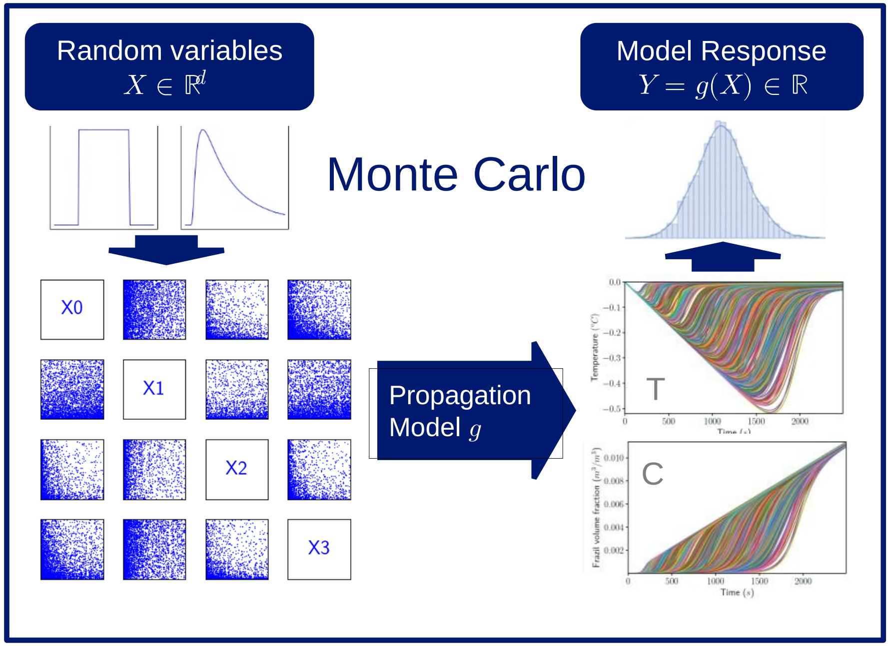
Parameter	Unit	Description	Category	Model	Uncertainty interval	PDF
C_0	-	Initial frazil volume fraction	Initial condition	Both	$[10^{-8}, 10^{-4}]$	Log-Uniform
r_0	m	Initial maximum radius	Initial condition	MSC	$[1.2 \times 10^{-4}, 2.1 \times 10^{-3}]$	Log-Uniform
r_{min}	m	Minimum radius	Discretization	MSC	$[10^{-6}, 10^{-4}]$	Log-Uniform
r_{max}	m	Maximum radius	Discretization	MSC	$[10^{-3}, 10^{-1}]$	Log-Uniform
$\overline{r}$	m	Mean radius	Discretization	SSC	$[1.2 \times 10^{-4}, 2.1 \times 10^{-3}]$	Log-Uniform
R	-	Diameter to thickness ratio	Source term ①	Both	$[5, 100]$	Uniform
δ_T	m	Thermal growth length scale	Source term ①	Both	$[7.34 \times 10^{-6}, 2.1 \times 10^{-3}]$	Log-Uniform
ε	$m^2.s^{-3}$	Turbulent dissipation rate	Source terms ①, ②	Both	$[10^{-9}, 1.5]$	Log-Uniform
α_T	-	Turbulent intensity	Source term ①	Both	$[0.01, 0.2]$	Log-Uniform
n_{max}	m^{-3}	Secondary nucleation efficiency cap	Source term ②	MSC	$[10^2, 10^8]$	Log-Uniform
τ_s	$m^{-2}.s^{-1}$	Seeding rate	Source term ②	Both	$[3 \times 10^{-1}, 10^4]$	Log-Uniform
a_f	s^{-1}	Flocculation coefficient	Source term ③	MSC	$[10^{-8}, 10^{-3}]$	Log-Uniform
a_d	-	Buoyancy coefficient	Source term ④	Both	$[0.086, 1.51]$	Uniform

C – UNCERTAINTY PROPAGATION

Principle of propagation with Monte Carlo

- Sampling of uncertain parameters (experimental design)
- Launching simulations (propagation)
- Characterization of output distributions (response) by moments (**mean, standard deviation, median, P05, P25, P75, P95**)

$$\widehat{\mu}_{Y^k} = \frac{1}{N}\sum_{j=1}^{N} y_j^k \quad \text{and} \quad \widehat{\sigma}_{Y^k} = \sqrt{\frac{1}{N}\sum_{j=1}^{N}\left(y_j^k - \widehat{m}_{Y^k}\right)^2}$$



Study cases

- Massively parallel computing: ~ 4 million simulations launched on the Cronos cluster
- 500,000 simulations on 960 proc = 24h of calculation time (for the MSC model) + 1h of post-processing
- Several Monte Carlo performed :

x8 Monte Carlo

Case	Model	Uncertain parameters	Case specificity	Sample size	No. of calls
1	SSC	$X = (C_0, \bar{r}, R, \varepsilon, \alpha_T)$	-	5×10^4	3.5×10^5
1b	SSC	$X = (C_0, \bar{r}, R, \varepsilon, \alpha_T)$	$\delta_T = r$	5×10^4	3.5×10^5
1c	SSC	$X = (C_0, \bar{r}, R, \delta_T, \varepsilon, \alpha_T)$	$\delta_T \in X$	5×10^4	4.8×10^5
2	MSC	$X = (C_0, r_0, R, \varepsilon, \alpha_T, n_{max}, a_f)$	-	5×10^4	4.5×10^5
2b	MSC	$X = (C_0, r_0, r_{min}, r_{max}, R, \varepsilon, \alpha_T, n_{max}, a_f)$	$r_{min}, r_{max} \in X$	6×10^4	6.6×10^5
2c	MSC	$X = (C_0, R, \varepsilon, \alpha_T, n_{max}, a_f)$	$r_0 = r_{min}$	5×10^4	4×10^5
3	SSC	$X = (C_0, \bar{r}, R, \varepsilon, \alpha_T, \tau_s, a_d)$	$\tau_s,\ a_d \in X$	7×10^4	6.3×10^5
4	MSC	$X = (C_0, r_0, R, \varepsilon, \alpha_T, n_{max}, \tau_s, a_f, a_d)$	$\tau_s,\ a_d \in X$	6×10^4	6.6×10^5

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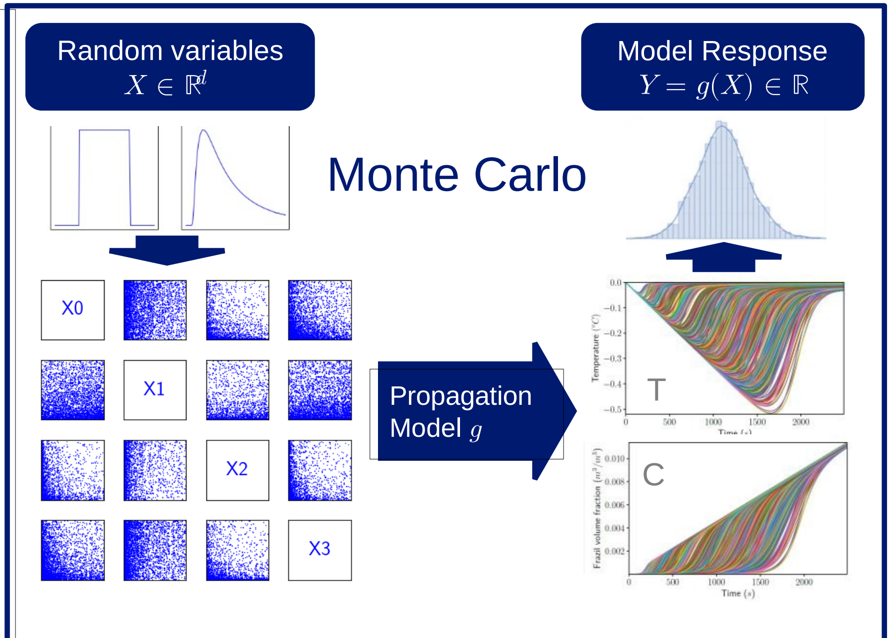
Principle of the sensitivity study

- Output variance decomposition method $Y = T$ or C

$$Var[Y^k] = \sum_{i=1}^{n_X} \underbrace{V_i(Y^k)}_{\mathrm{Var}[\mathbb{E}[Y^k|X^i]]} + \sum_{i<j} V_{ij}(Y^k) + \cdots + V_{1\ldots n_X}(Y^k),$$

$k \rightarrow$ **Time index /** $i \rightarrow$ **Index of the uncertain variable** X_i

- **Sobol indices (Time series):** between 0 and 1, sum = 1
- **Aggregate Sobol Indices:** Time Integration



Sobol indices

First order Sobol index relative to X_i : $S_i^k = \dfrac{V_i(Y^k)}{\mathrm{Var}[Y^k]}$

If large, then the i-th factor alone strongly influences the variability of the output

Total Sobol relative to X_i :

$$ST_i^k = S_i + \sum_{i \neq j} S_{ij} + \sum_{i\neq j, k\neq i, j\leq k} S_{ijk} + \cdots$$

= Sum of all indices relating to Xi

Aggregate Sobol relating to X_i : $AS_i = \dfrac{\sum_{k=1}^{n_t} V_i(Y^k)}{\sum_{k=1}^{n_t} \mathrm{Var}[Y^k]}$

C – UNCERTAINTY PROPAGATION

Moments : **case without buoyancy**

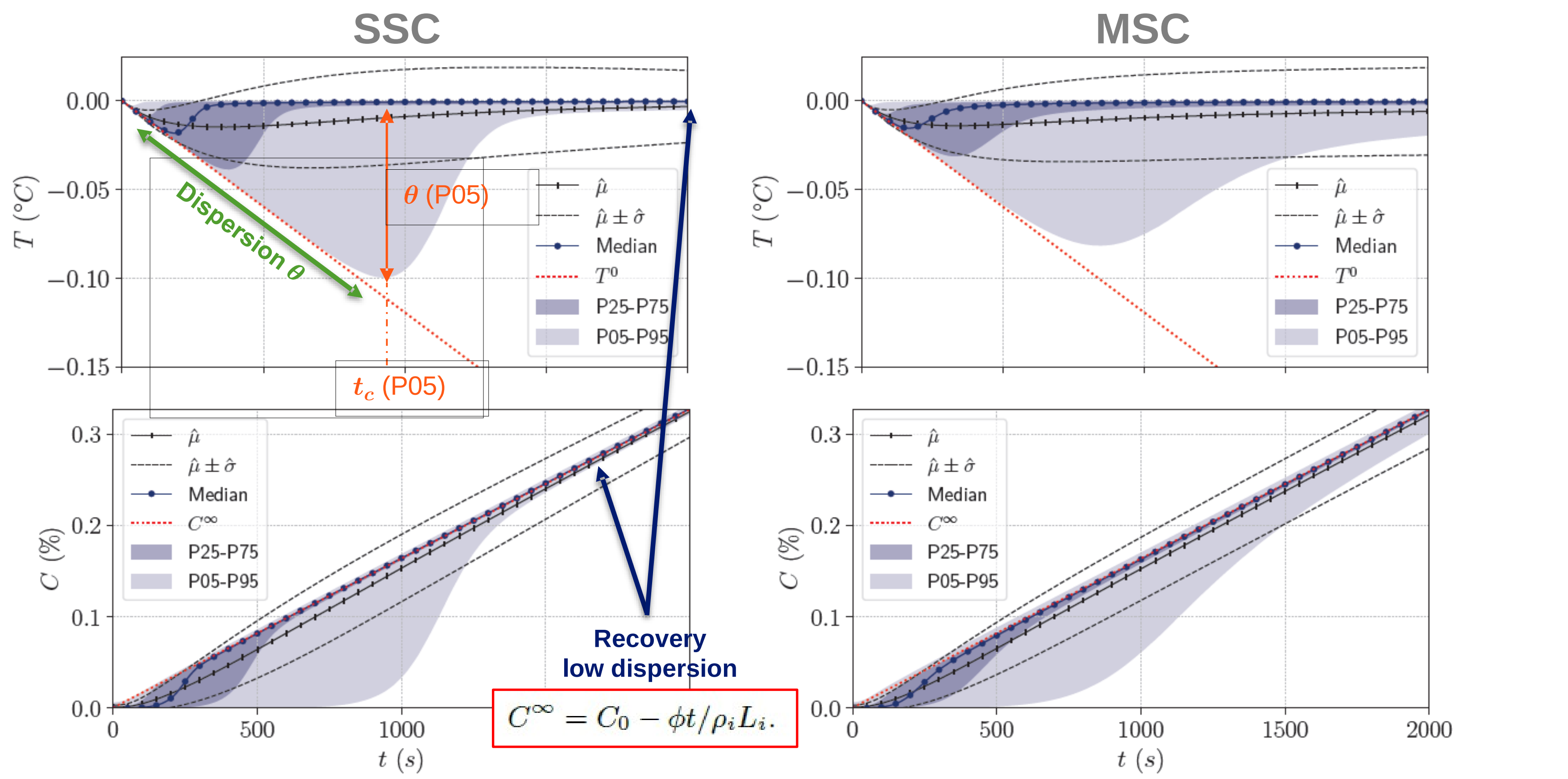


FIGURE 5 – Uncertainty propagation results for SSC (case 1) on the left and MSC (case 2) on the right : mean, standard deviation, median, 5^{th}, 25^{th}, 75^{th} and 95^{th} percentiles are computed for $t_k(0 \leq k \leq n_t)$.

C – UNCERTAINTY PROPAGATION

Sobol indices: **case without buoyancy**

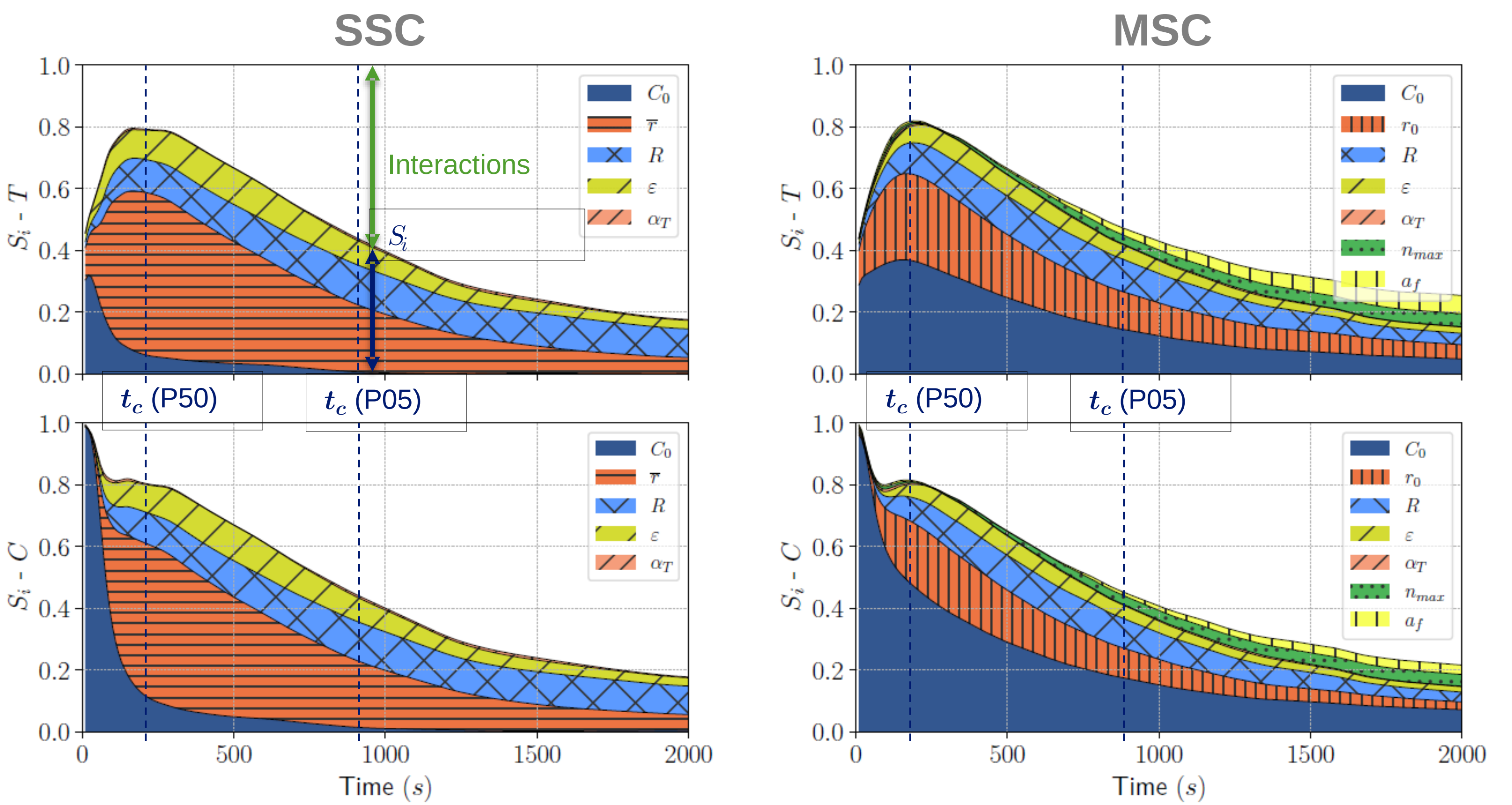


FIGURE 6 – Time series of first-order Sobol indices (S_i) for temperature (T) and total frazil volume fraction (C) for SSC (case 1) on the left and MSC (case 2) on the right.

C – UNCERTAINTY PROPAGATION

Moments : **case with buoyancy**

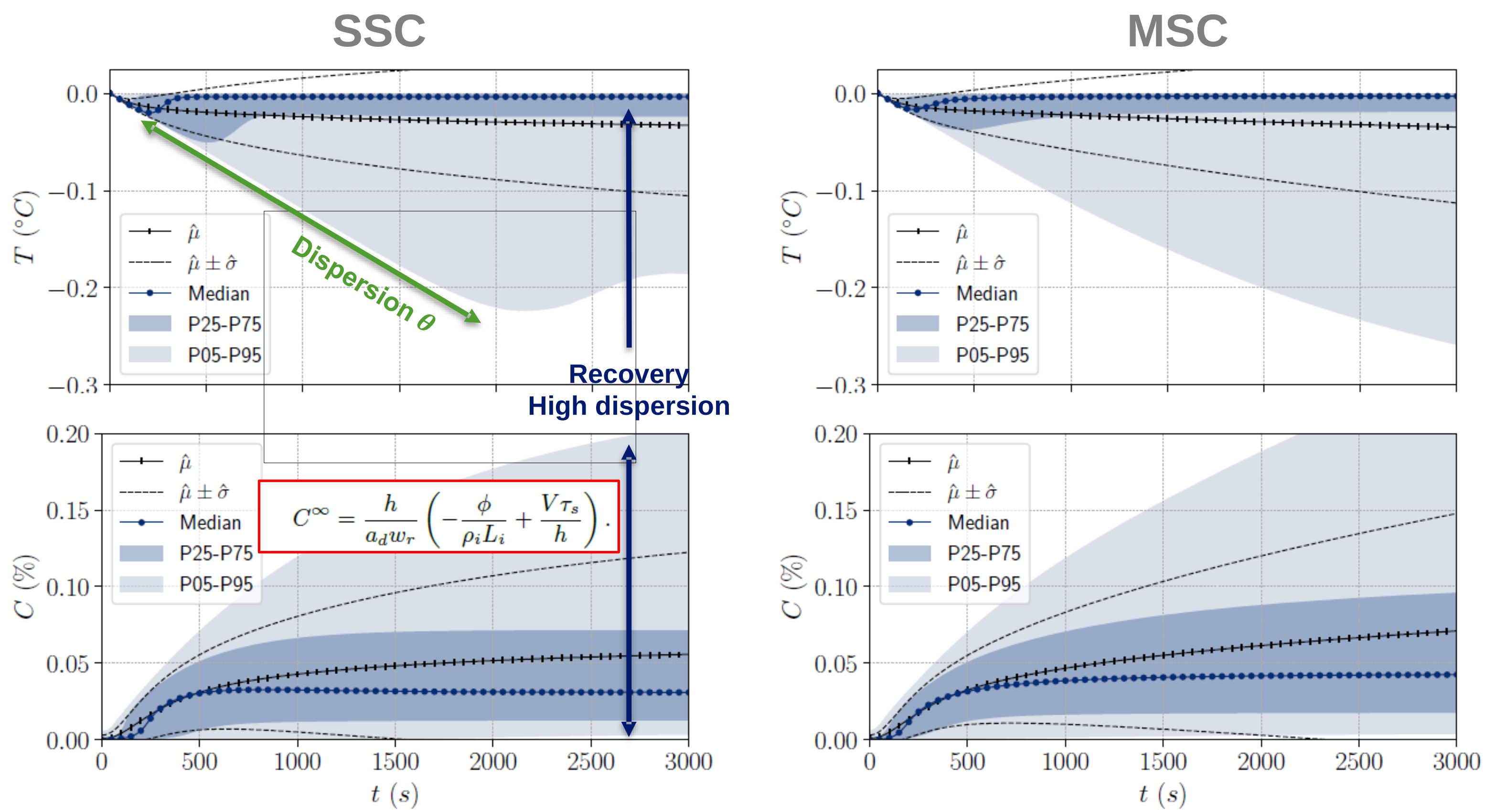
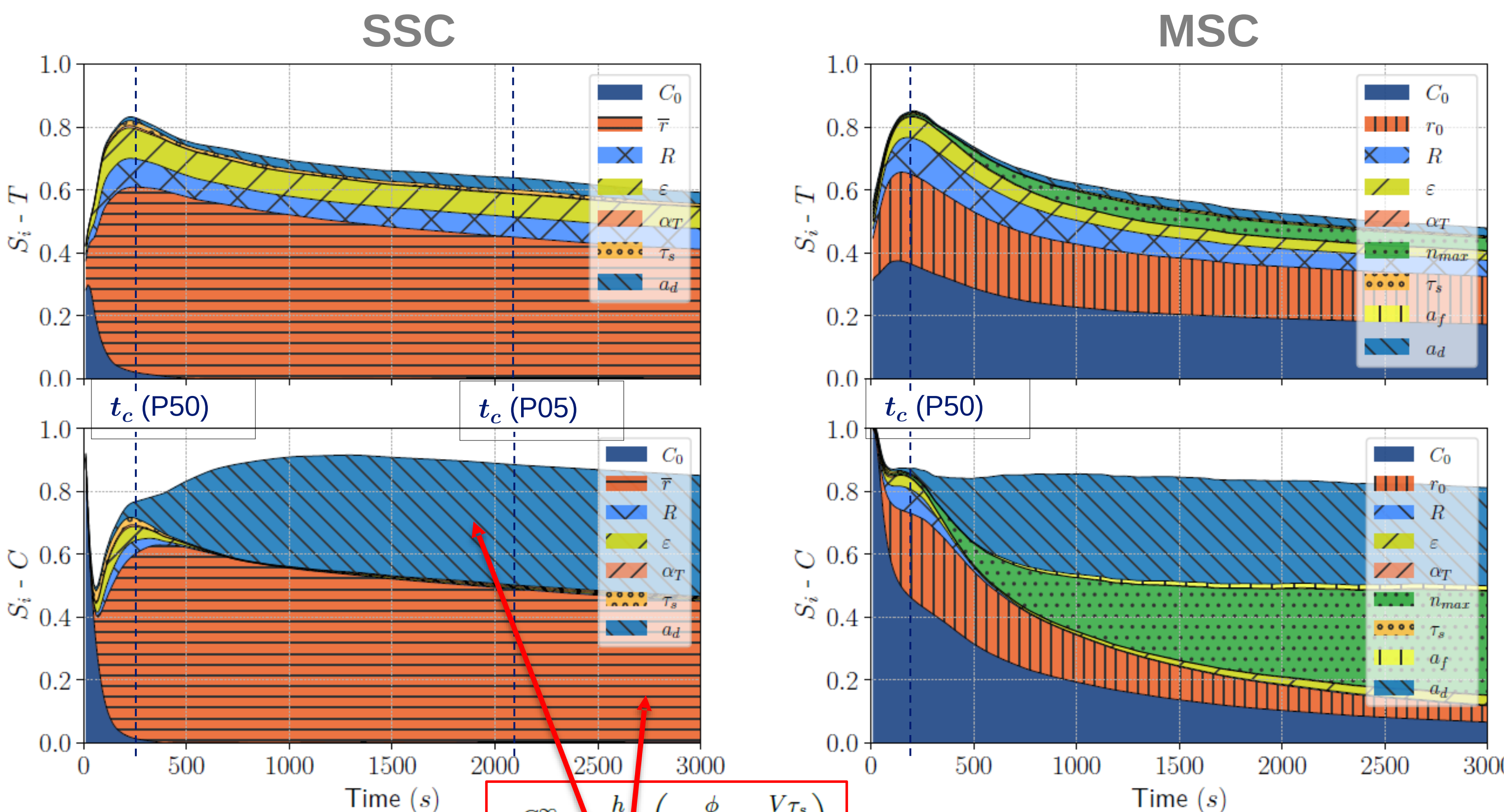


FIGURE 8 – Uncertainty propagation results for SSC (case 3) on the left and MSC (case 4) on the right : mean, standard deviation, median, 5^{th}, 25^{th}, 75^{th} and 95^{th} percentiles computed for $t_k (0 \le k \le n_t)$.

C – UNCERTAINTY PROPAGATION

Sobol indices: **case with buoyancy**



$$C^{\infty} = \frac{h}{a_d w_r}\left(-\frac{\phi}{\rho_i L_i} + \frac{V\tau_s}{h}\right).$$

FIGURE 9 – Time series of first-order Sobol indices (S_i) for temperature (T) and total frazil volume fraction (C) for SSC (case 3) on the left and MSC (case 4) on the right.

C – UNCERTAINTY PROPAGATION

Summary of cases : aggregated Sobol indices

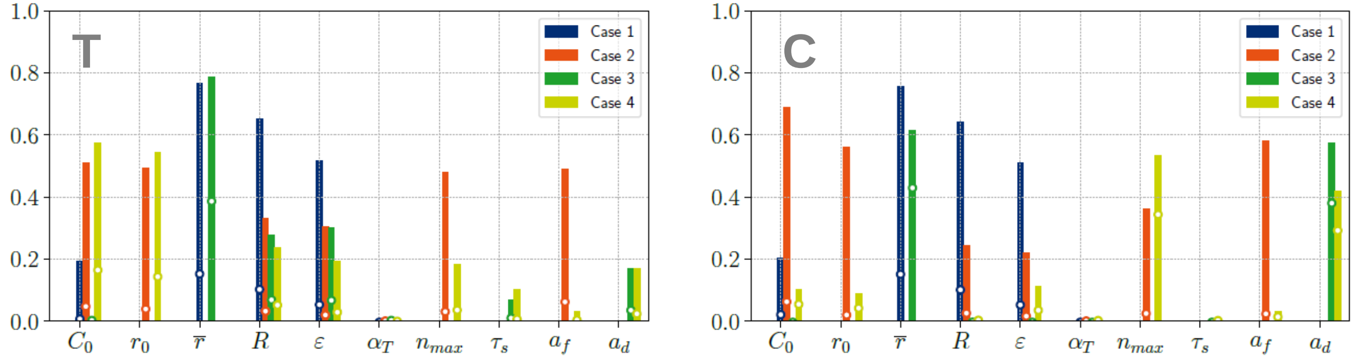


FIGURE 7 – Aggregated first order Sobol indices (dots) and aggregated total Sobol indices (bars) for temperature (T) and total frazil volume fraction (C) for cases (1), (2), (3) and (4).

C – UNCERTAINTY PROPAGATION

Influence of the cooling rate of the water body

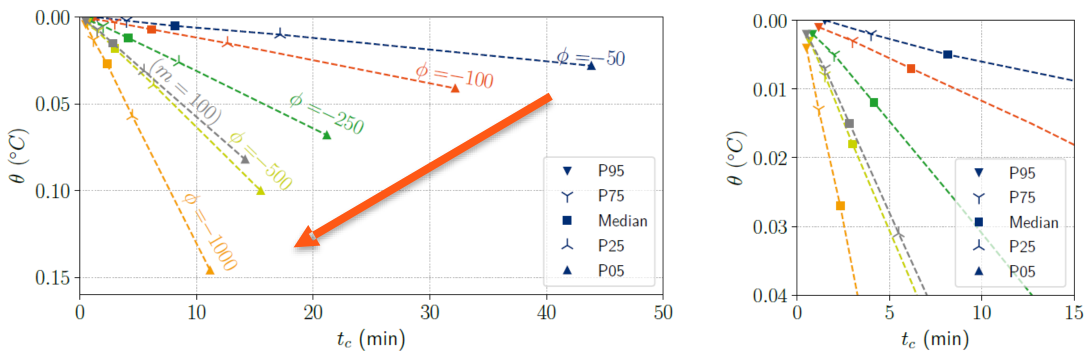
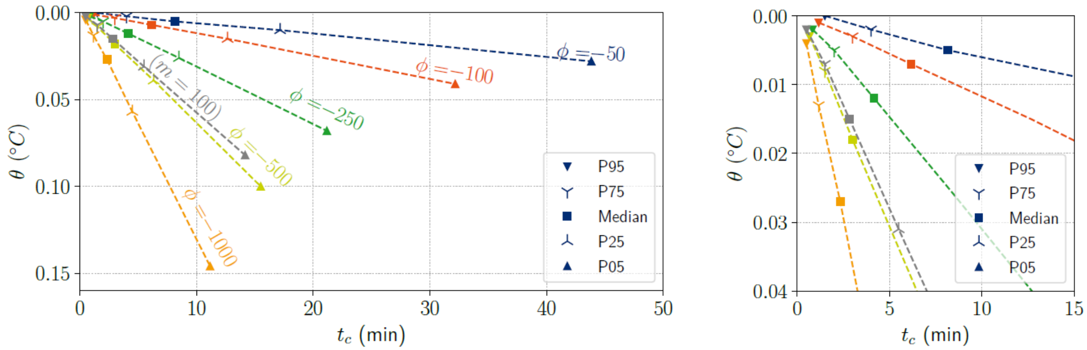


FIGURE 10 – Maximum supercooling point scatter computed from median, 5^{th}, 25^{th}, 75^{th} and 95^{th} percentile time series at different cooling rates ($\phi = -50, -100, -250, -500$, and -1000 W.m^{-3}) for case (1) and with $\phi = -500$ W.m^{-3} for case (2).

Transfer of dispersion time to maximum supercooling dispersion (relationship duration x intensity)

C – UNCERTAINTY PROPAGATION

Influence of the cooling rate of the water body



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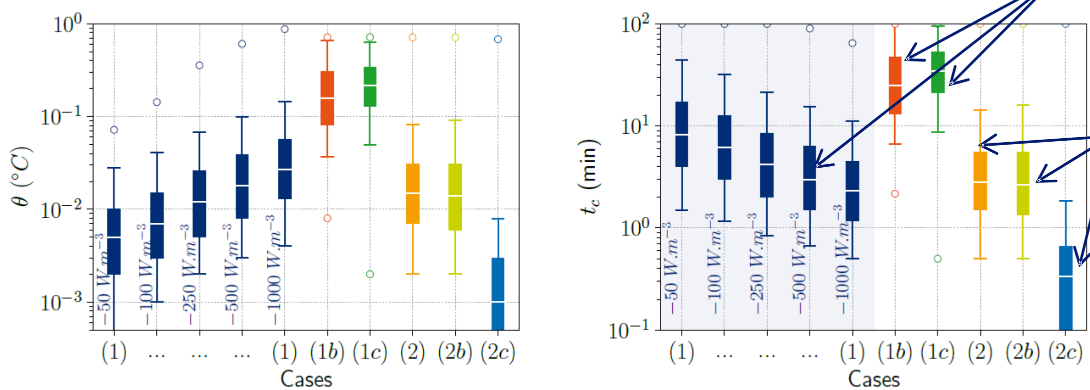
Summary of the different Monte Carlo simulations



Different "scaling" for the turbulent boundary layer around the crystals

Bad scaling (r instead of e)
=> factor 100 on G !!!

Different initializations of the MSC model

Considerable impact on transient dispersion

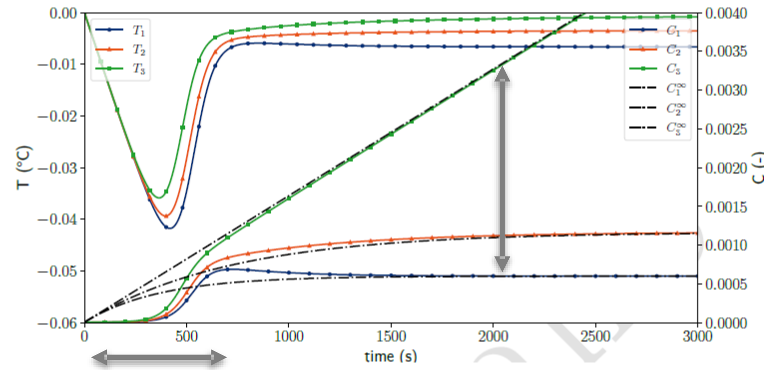
FIGURE 11 – Maximum supercooling point scatter computed from median, 5^{th}, 25^{th}, 75^{th} and 95^{th} percentile time series at different cooling rates ($-50, -100, -250, -500$, and -1000 W.m^{-3}) for case (1), comparison between the choice of the length scale δ_T (cases 1b and 1c) and comparison between different initial conditions (cases 2b and 2c).

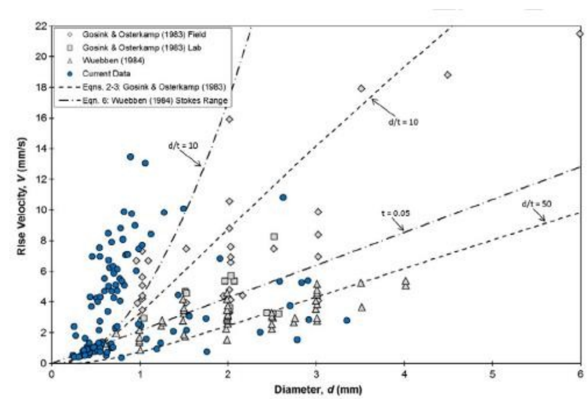
SOMMAIRE ✦

CONCLUSION

Main study conclusions

- **Choice of frazil model → SSC**
  - MSC is very expensive :
    - – Time conditioned by the smallest radius (dt≤0.25 s)
    - – High number of classes to achieve convergence (m≥ 100)
  - Similar dispersion between MSC and SSC
- **Time scale and most influential parameters**
  - **Transient**: CI + discretization of radius space
  - **Asymptotic**: buoyancy velocity + cooling rate
- **Importance of buoyancy**
  - Neglecting wr is extremely penalizing
  - Choice of law that minimizes wr (Morse and Richard 2009)





Perspectives

- **Poor description of input distribution** because of the **lack of data** (more field and laboratory work is required)
- **Dependency** between input variables should be investigated
- **Optimal calibration** of models using OpenTURNS and ADAO is ongoing

Study published in The Cryosphere "Uncertainty analysis of single- and multiple-size-class frazil ice models" F. Souillé, C. Goeury, and R.-S. Mouradi

OpenTURNS allowed simple uncertainty analysis thanks to its ease of use and well thought documentation

THANK YOU