The 33th Annual symposium of the Israeli section of the combustion institute.

Onset of Nucleate Boiling due to Rapid Heating – How does it relate to Combustion?

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Research Aim

Predicting the nucleation temperature due to an isobaric process under moderate to high heating rates for different liquids.

Outline

Aim & Motivation

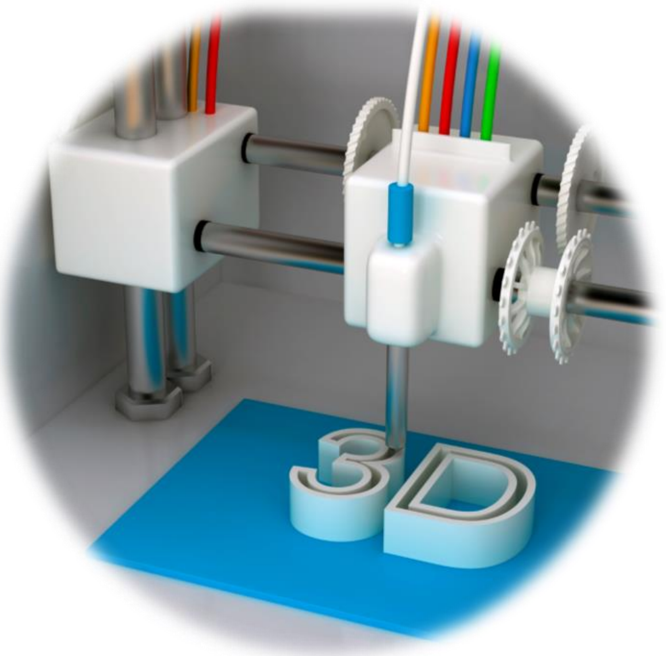
Phase-Change Thermodynamics

Rapid Isobaric heating

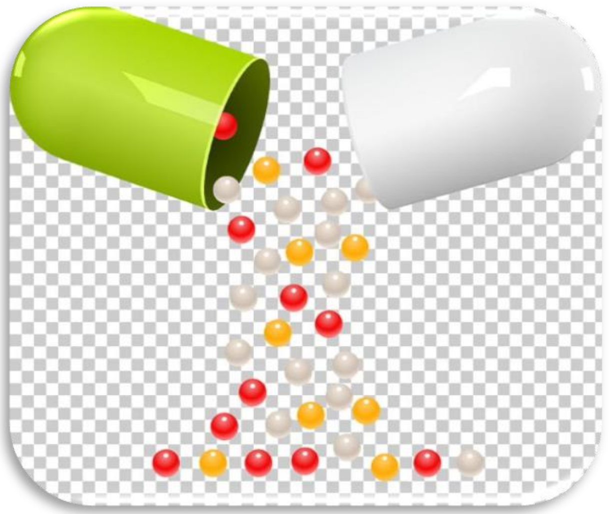
Model

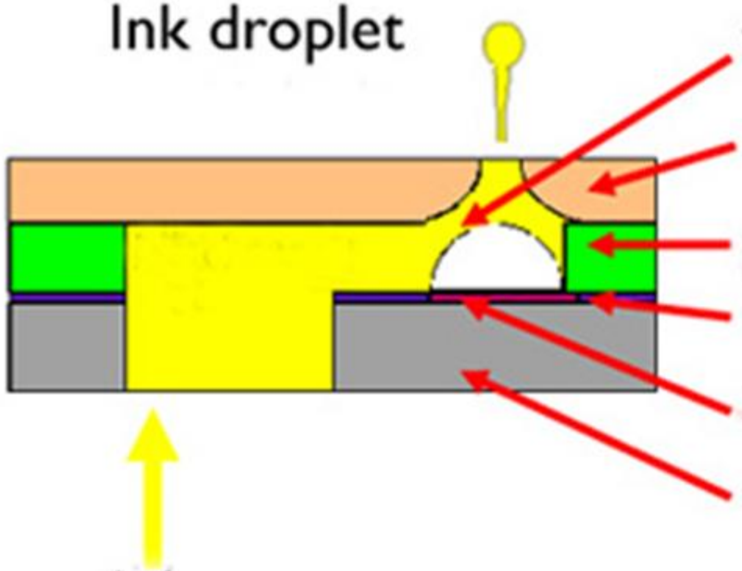
Results

Conclusions



ONB & Industry





Ink droplet

Vapor bubble

Orifice plate

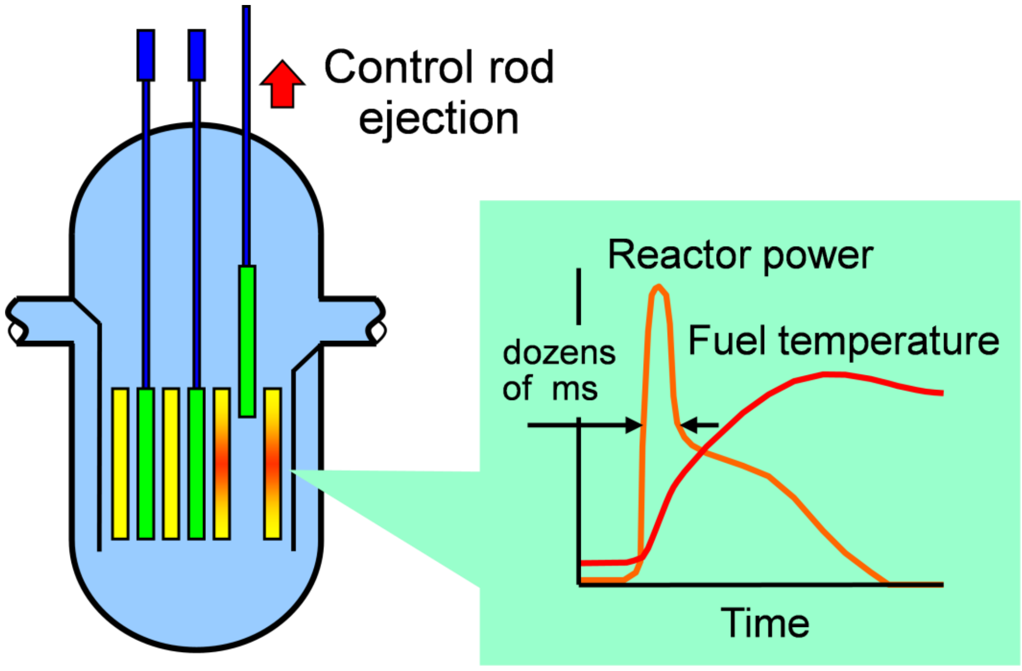
Photoimageable polymer

Thin film conductor

Thin film resistor

Silicon substrate

Ink



Control rod ejection

Rapid rises of power and fuel temperature

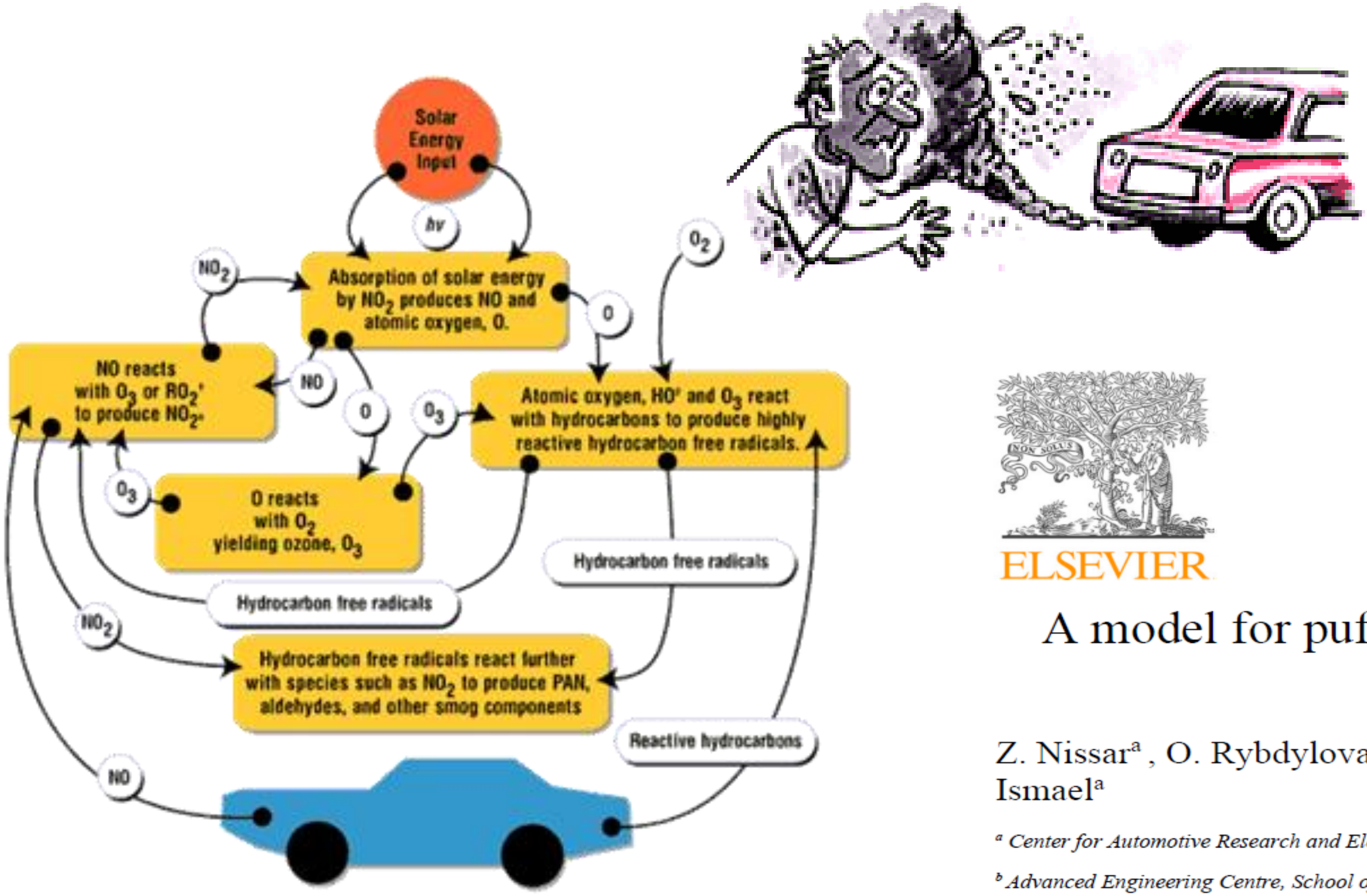
Intertwining Boiling & Combustion **Promotion**

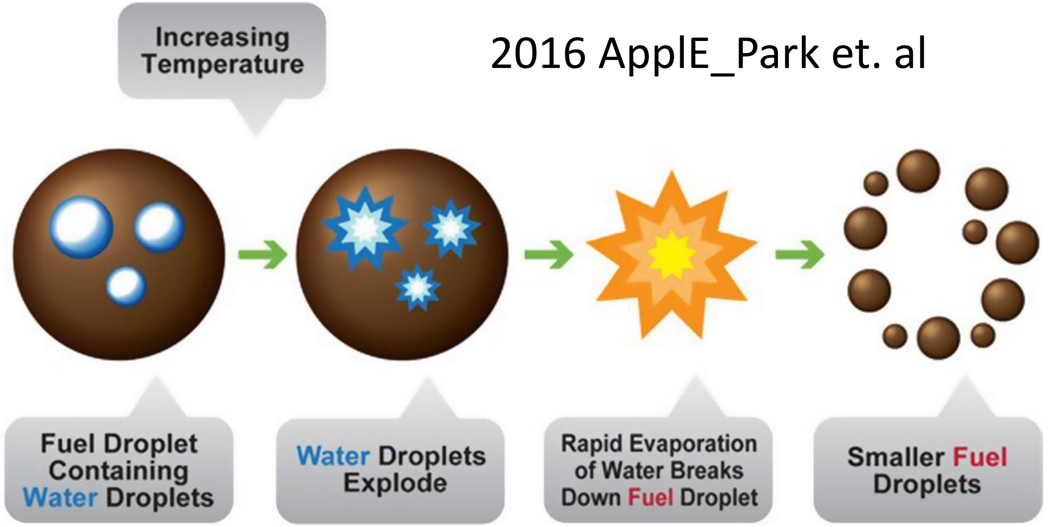
Fuel Drop on Hot Engine wall

Unburnt HC

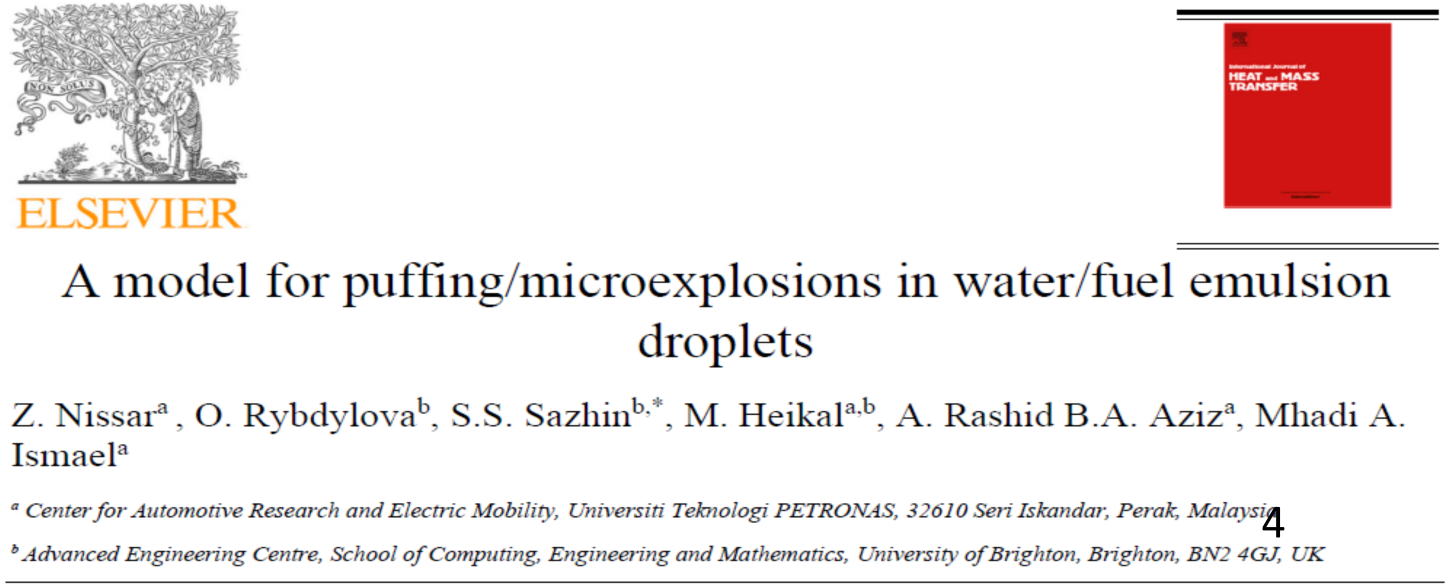
Reactive HC

PAN, Aldehydes Smog





2016 ApplE_Park et. al



ELSEVIER

A model for puffing/microexplosions in water/fuel emulsion droplets

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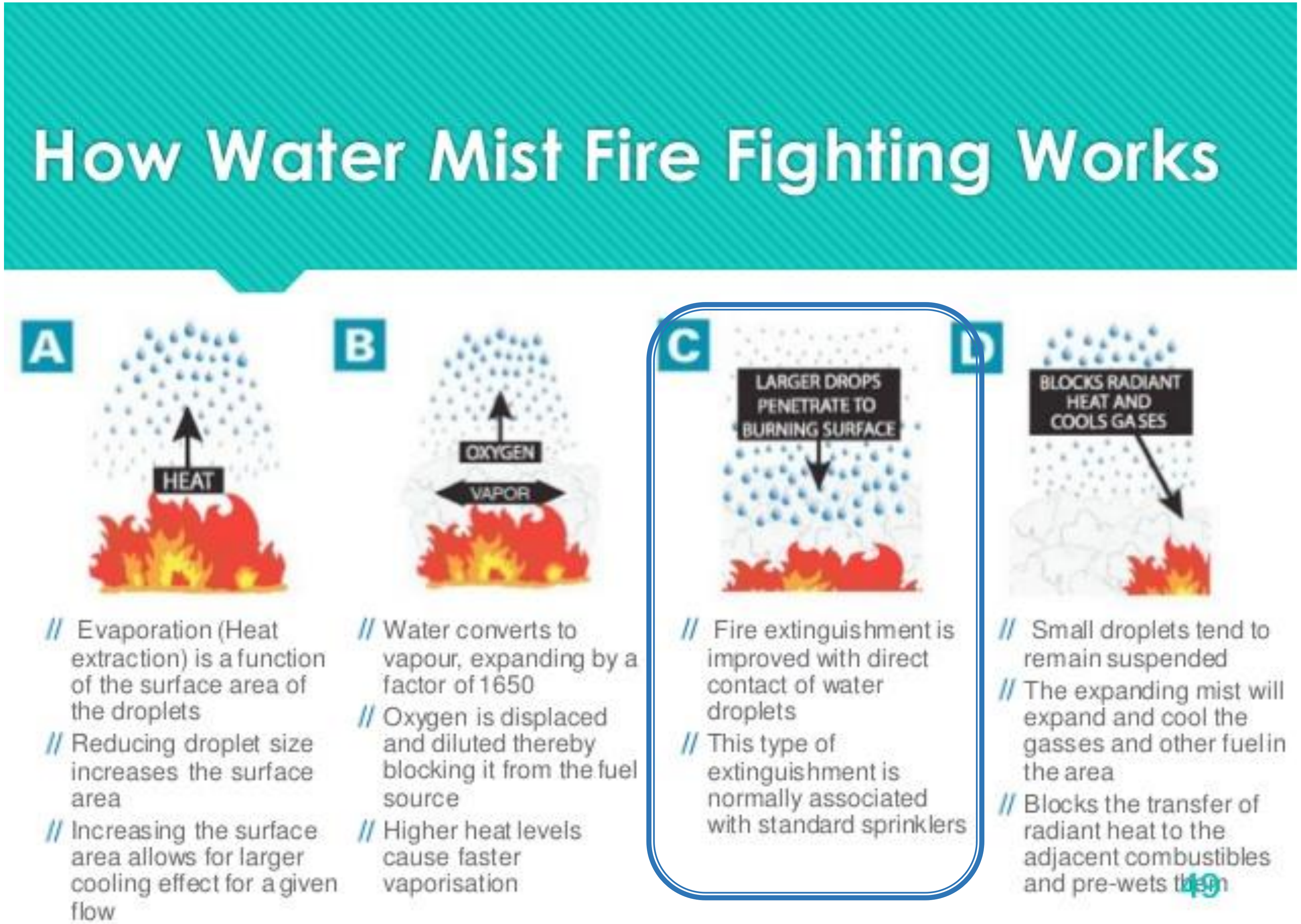
Intertwining Boiling & Combustion Suppression



How Water Mist Fire Fighting Works

A

- Evaporation (Heat extraction) is a function of the surface area of the droplets
- Reducing droplet size increases the surface area
- Increasing the surface area allows for larger cooling effect for a given flow

B

- Water converts to vapour, expanding by a factor of 1650
- Oxygen is displaced and diluted thereby blocking it from the fuel source
- Higher heat levels cause faster vaporisation

C

- Fire extinguishment is improved with direct contact of water droplets
- This type of extinguishment is normally associated with standard sprinklers

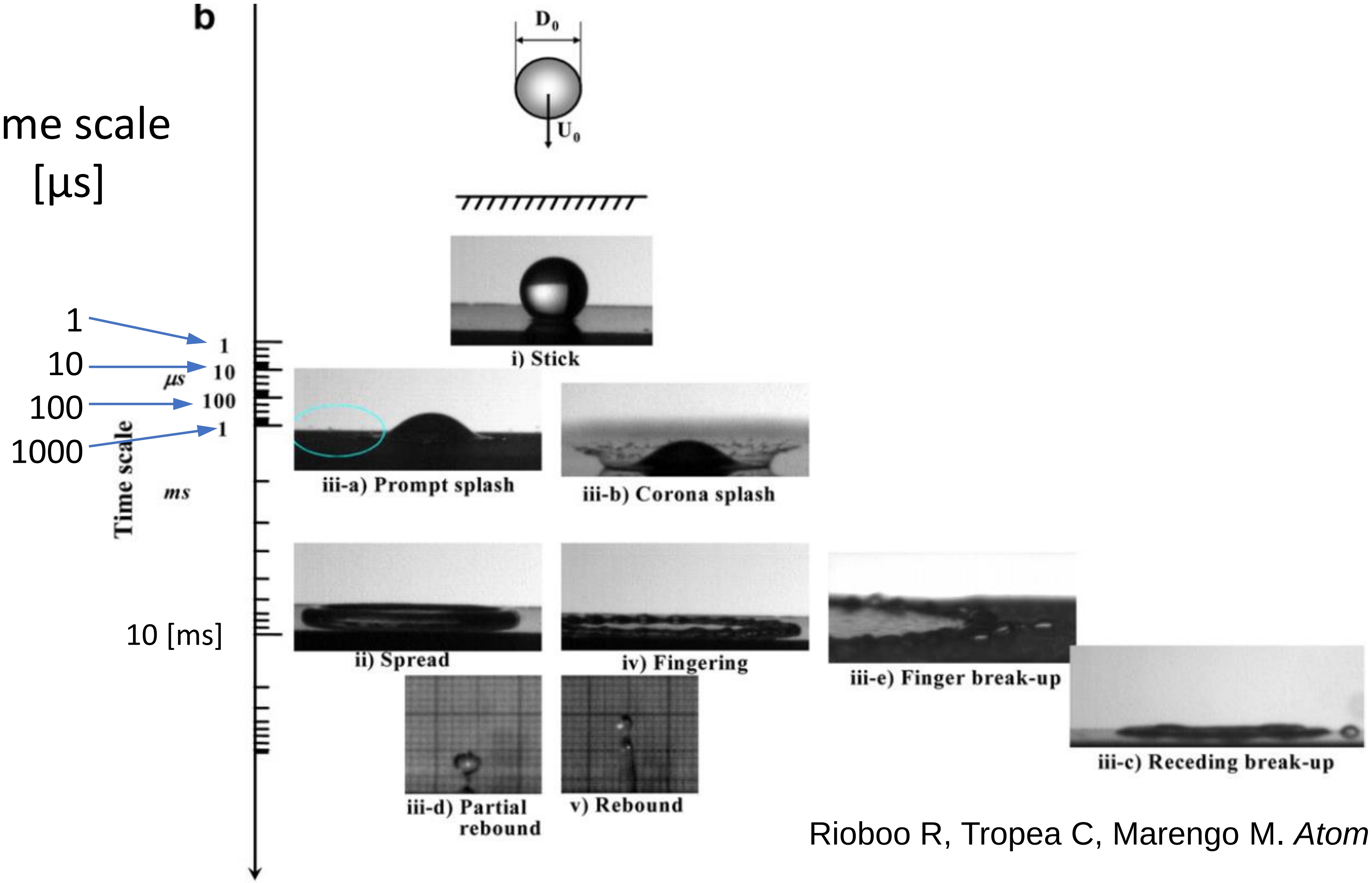
D

- Small droplets tend to remain suspended
- The expanding mist will expand and cool the gasses and other fuel in the area
- Blocks the transfer of radiant heat to the adjacent combustibles and pre-wets them

https://www.slideshare.net/s

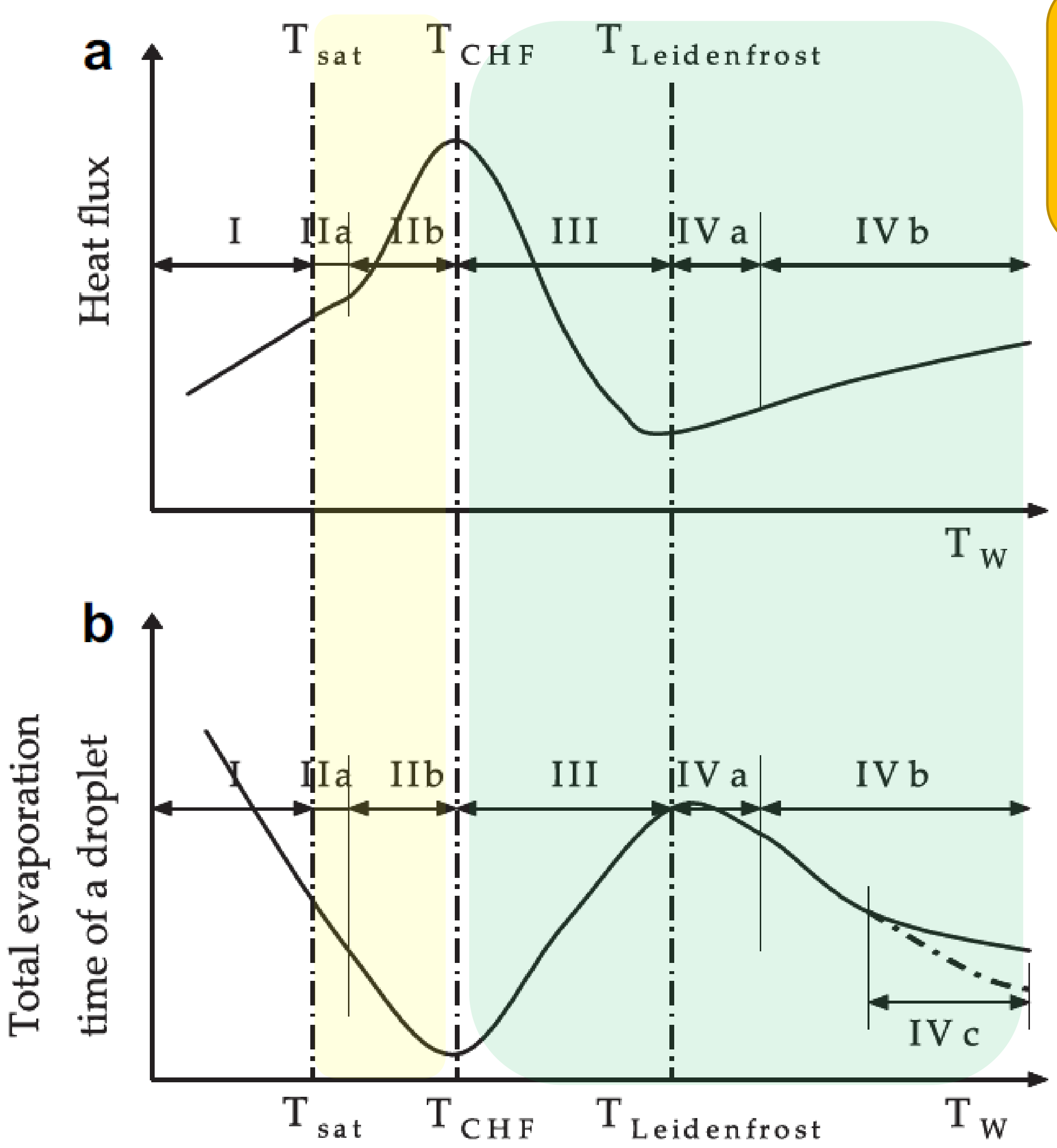
Drop impact - Isothermal flat, dry surfaces

Time scale
[µs]

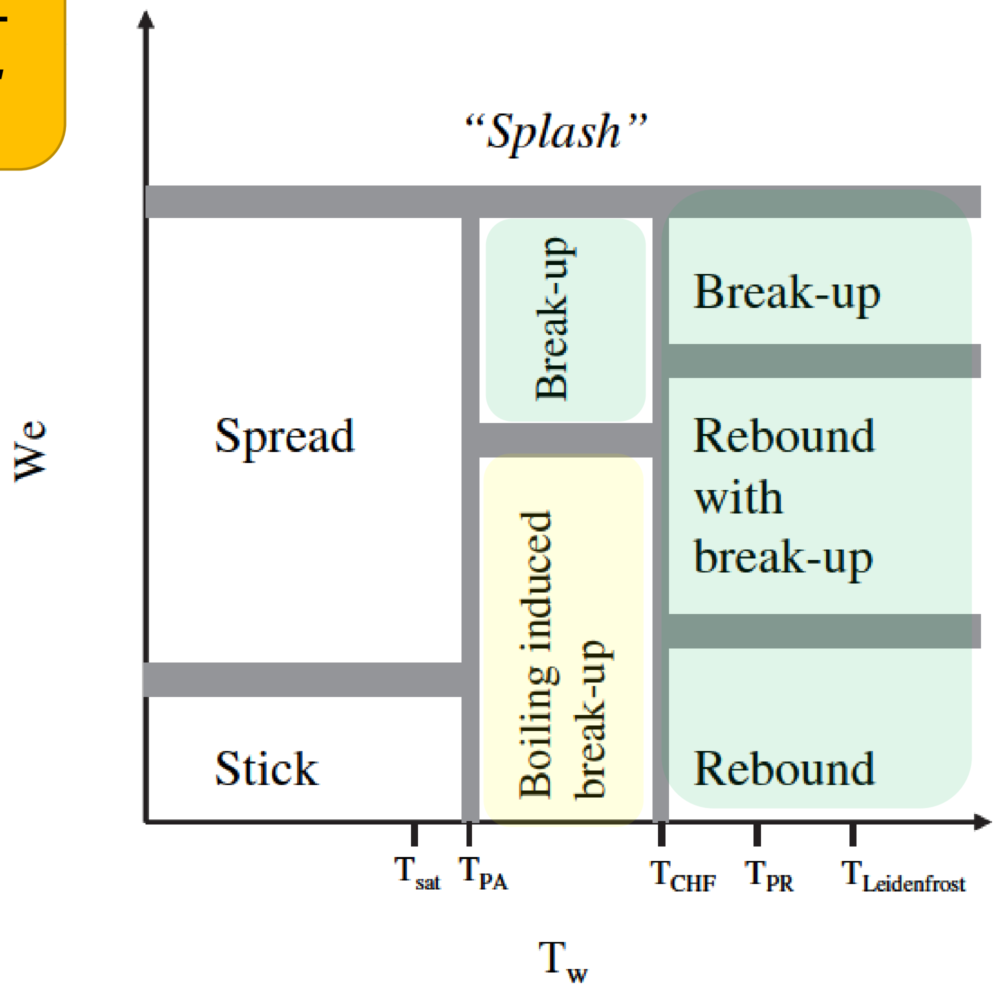


Rioboo R, Tropea C, Marengo M. *Atom Sprays* (2001)

Fuel-drop impact onto - heated, dry surfaces

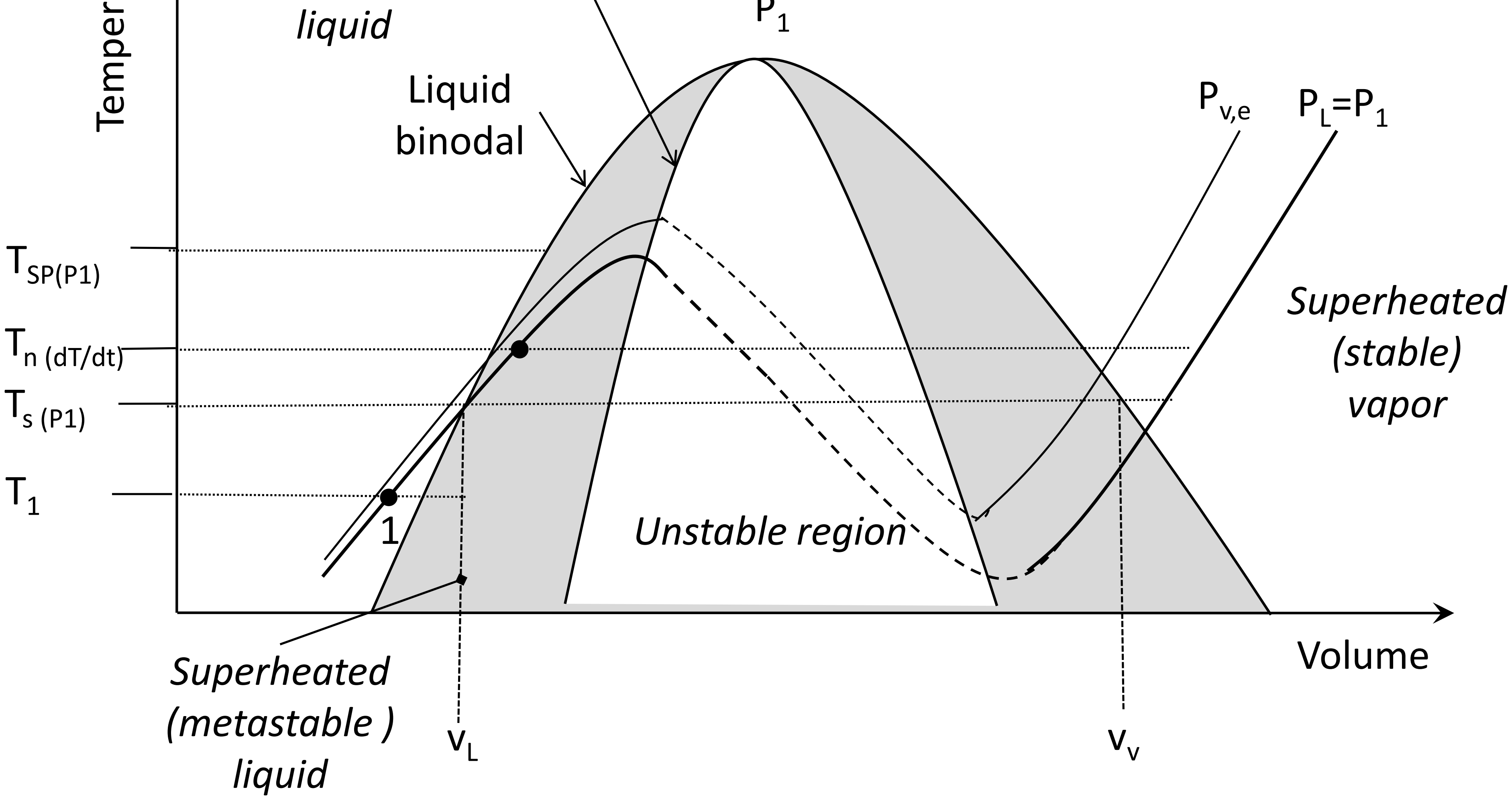


$$\frac{\tau_{HT}}{\tau_{MomT}}$$



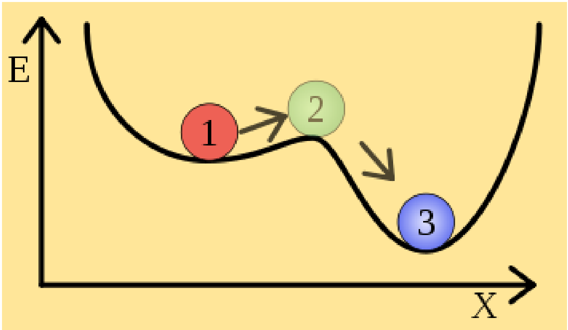
Moreira, Moita & Panao, *PECS* (2010)

Metastable liquids



$$\int_0^{\tau_m[T(t)]} J[T(t)]dt < 1$$

Metastability denotes the phenomenon when a system spends an **extended time** in a configuration other than the system's state of least energy



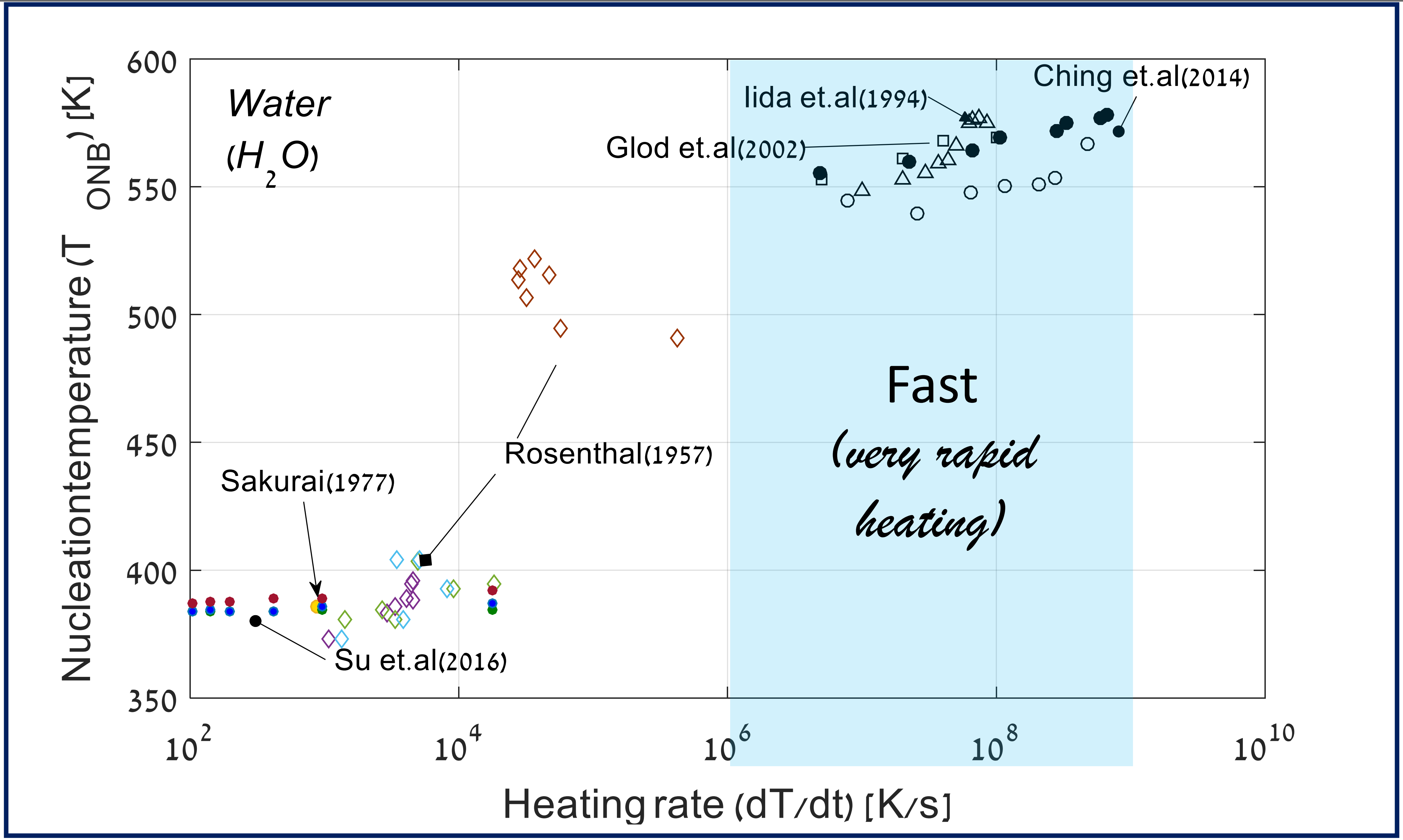
https://commons.wikimedia.org/wiki/File:Meta-stability.svg

?

So, if given an *initial pressure* & a *heating rate*, could you predict the *nucleation temperature*?

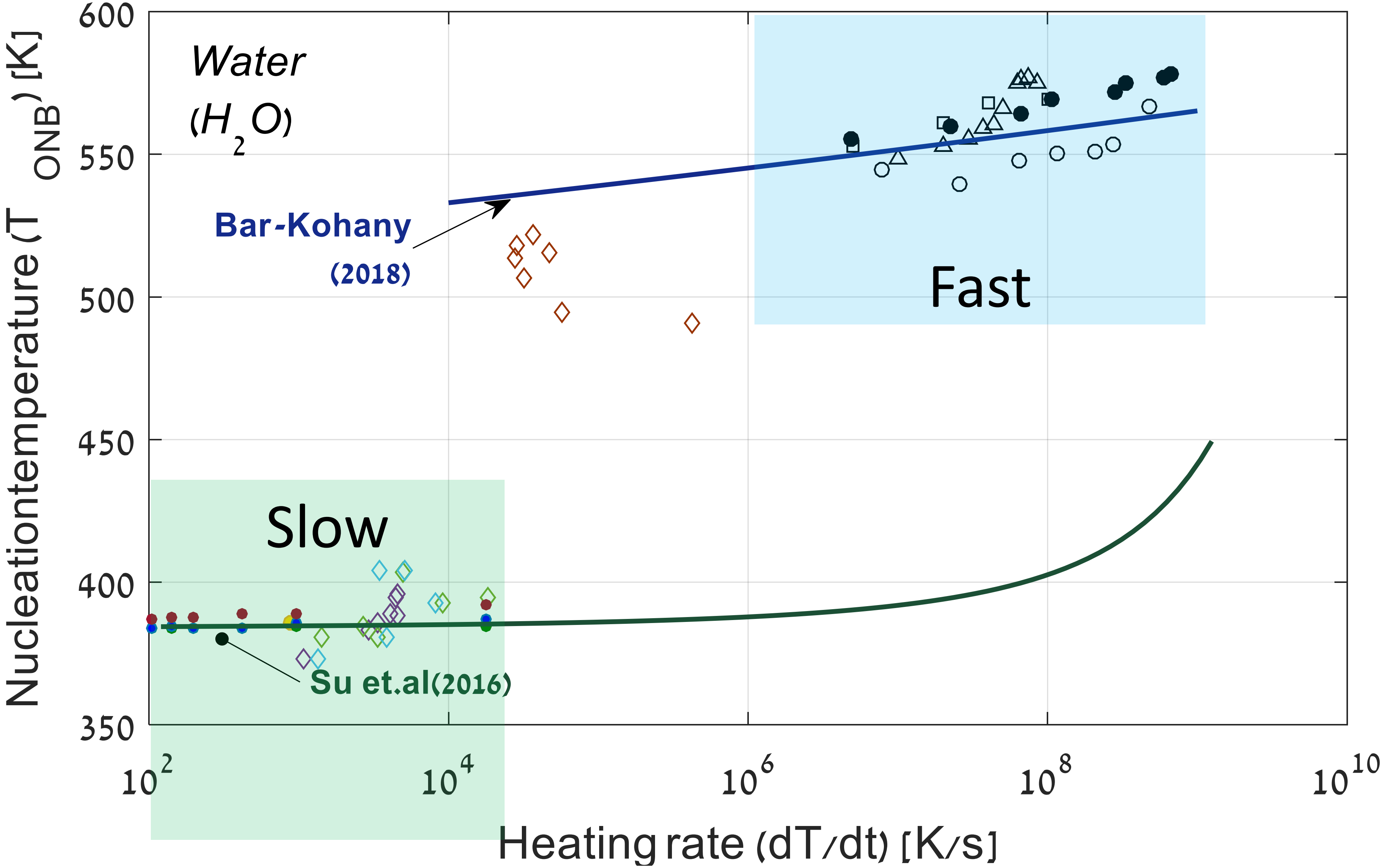
Nucleation Pathways

Rapid Isobaric heating (p=1 atm)



Nucleation Pathways

Rapid Isobaric heating (p=1 atm)



Classic Thermodynamic potentials – Gibbs no.

$$\frac{G_b}{\phi} \equiv \frac{W_c}{k_B T} = \frac{16\pi\sigma^3}{3k_B T\left(P_L - P_{v,e}\right)^2} \quad \Rightarrow \boxed{\Delta P_n = P_L - P_{v,e} = \sqrt{\frac{1}{\frac{G_b}{\phi}} \frac{16\pi\sigma^3}{3k_B T\left(1 - \frac{\rho_v}{\rho_L}\right)}}}$$

Dynamic **Thermodynamics**

Bartak (IJMF,1990), rapid depressurization

$$\frac{G_b}{\phi} \equiv \tilde{f}_1(p_0, T_0)\tilde{f}_2(\dot{T})\tilde{f}_3(\Sigma)$$

$$\Rightarrow \quad \Delta P_n = P_L - P_{v,e} = \sqrt{\frac{1}{\tilde{f}_1(p_0, T_0)\tilde{f}_2(\dot{T})\cancel{\tilde{f}_3}(\Sigma)} \frac{16\pi\sigma^3}{3k_B T\left(1 - \frac{\rho_v}{\rho_L}\right)}}$$

$\tilde{f}_3 \rightarrow 1$ (isobaric process)

Aim & Motivation

Phase-Change Thermodynamics

Rapid Isobaric heating

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Clausius-Clapeyron

$$\frac{P_L - P_{v,e}}{T_n - T_L} = \frac{\Delta P_n}{\Delta T_n} \approx \frac{h_{fg}}{T_s \Delta v}$$

$$\Delta T_n = T_n - T_L = \frac{\Delta P_n T_s (v_v - v_L)}{h_{fg}} = f_1(P_0) f_2(\dot{T}) \overbrace{\frac{v_v}{h_{fg}} \sqrt{\frac{16\pi\sigma^3 T_s}{3k_b}}}^{\Delta T_{S\,(Ps(T_0))}}$$

$$f_j = \sqrt{\frac{1}{\tilde{\mathrm{f}}_j}}$$

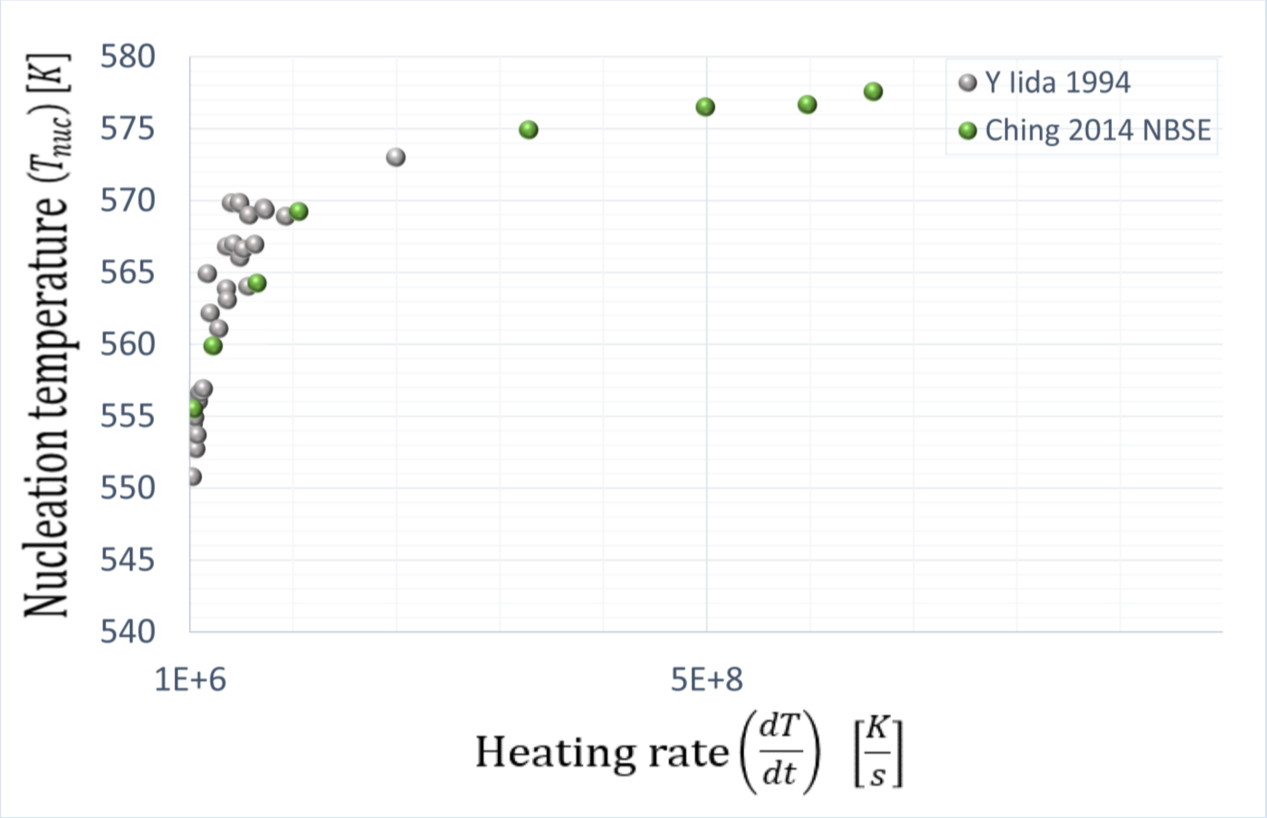
Thermodynamic model - $f_2(\dot{T})$

T↑ ⇒ J↑; Local heterophase fluctuations produce short-range order heterogeneity

⇒ $\dot{T}$ depends on the temporal evolution of the temperature.

$$f_2(\dot{T}) \propto \dot{T}^{\frac{c}{Ja}}$$

$$\mathrm{Ja} \equiv \frac{\rho_L}{\rho_v} \frac{C_{P,L}\,(T - T_S)}{h_{fg}}$$



Bar-Kohany T. and Amsalem Y., Int. J. Heat Mass Transf., 2018

Thermodynamic model - f_1

$$\left.\dot{T} \to 0\right\} \begin{array}{l} T_n \to T_s \\ f_2(\dot{T}) \to 1 \end{array}$$

$$\Delta T_n = f_1(P_0) f_2(\dot{T}) \Delta T_S$$

$$\boxed{f_1(P_L) \propto \frac{T_S}{\Delta T_S}}$$

$$\boxed{f_2(\dot{T}) \propto \dot{T}^{\frac{c}{Ja_{HN}}}}$$

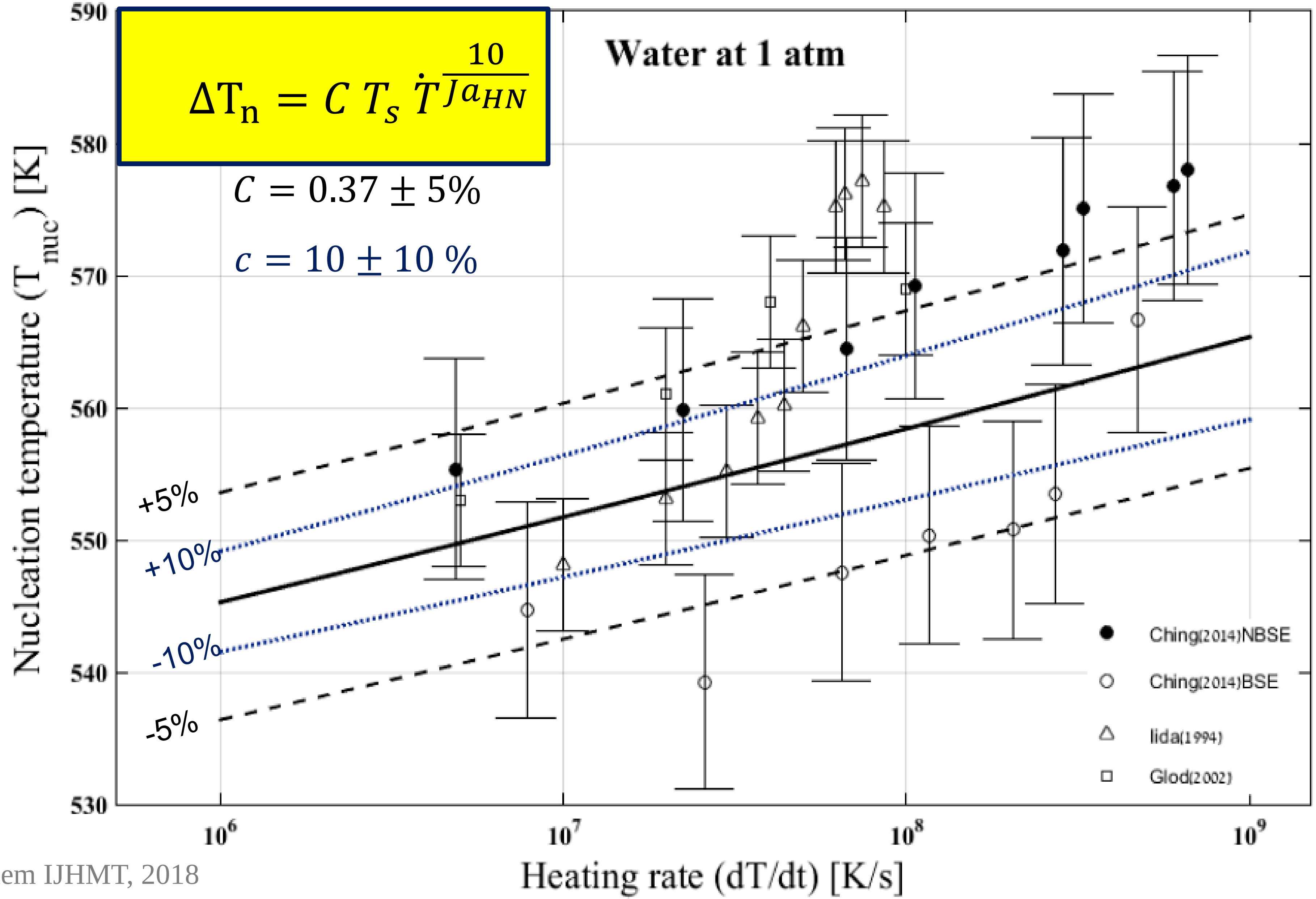
Universal Correlation

$$\Delta \mathrm{T_n} = f_1(P_0) f_2(\dot{T}) \Delta \mathrm{T_S};$$

$$\boxed{\Delta \mathrm{T_n} = C\, T_s\, \dot{T}^{\frac{10}{Ja_{HN}}}}$$

Bar-Kohany T. and Amsalem Y., Int. J. Heat Mass Transf., 2018

Correlation vs. Experimental results - Water



$$\Delta T_n = C\, T_s\, \dot{T}^{\frac{10}{Ja_{HN}}}$$

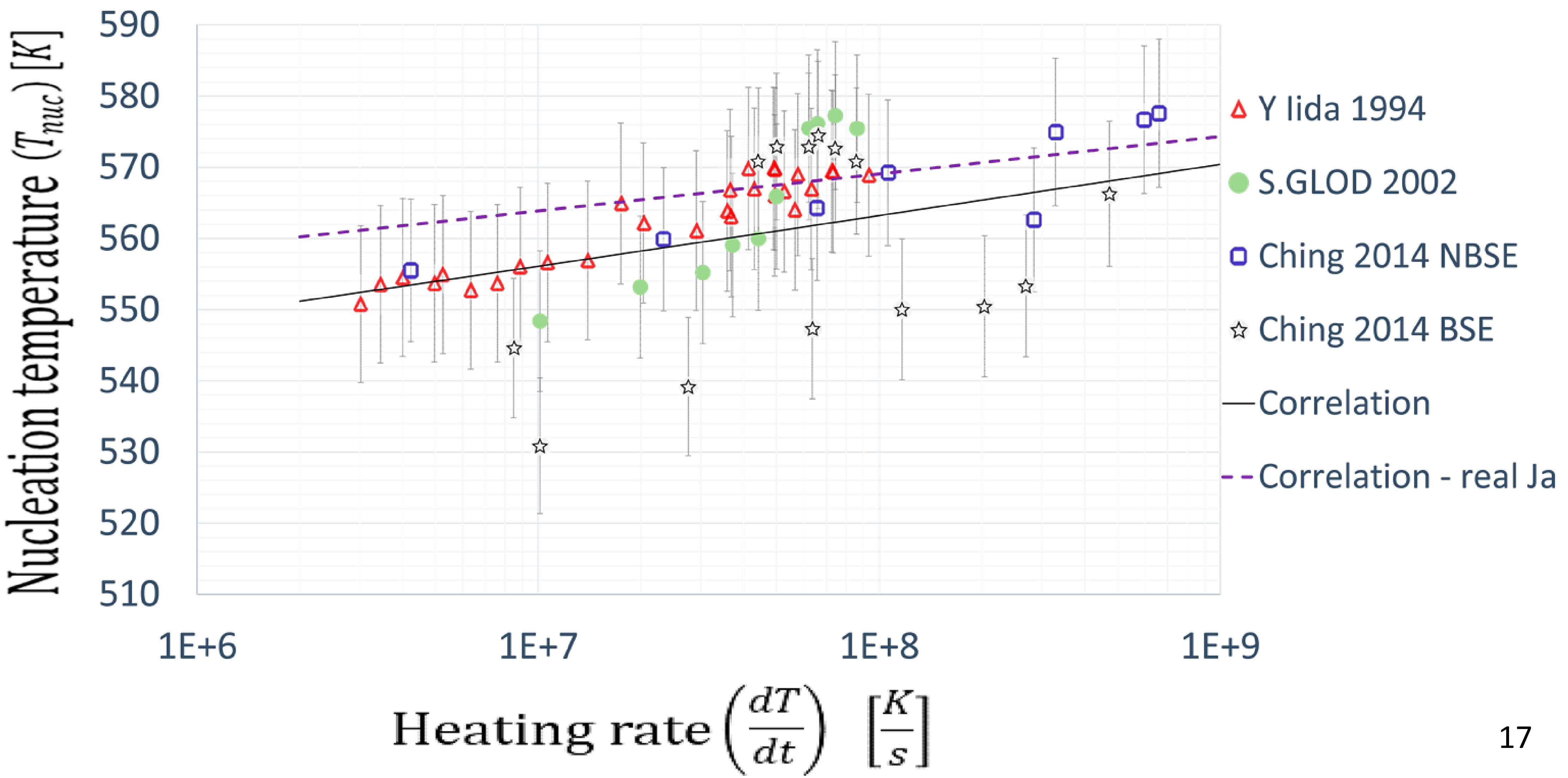
$C = 0.37 \pm 5\%$

$c = 10 \pm 10\ \%$

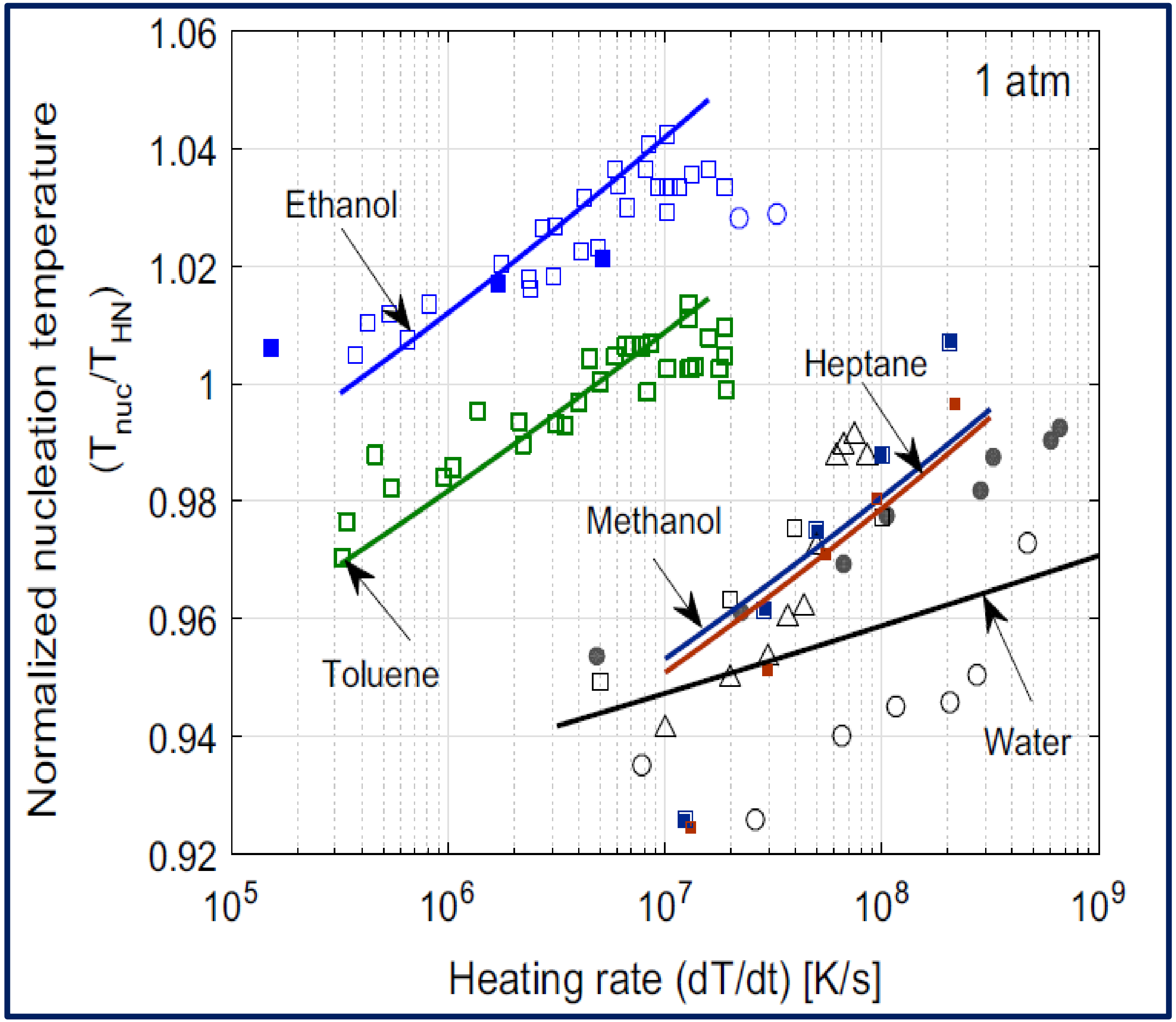
Bar-Kohany & Amsalem IJHMT, 2018

Universal Correlation

$$T_n = CT_s\dot{T}^{\frac{c}{Ja(T_n)}} + T_s \approx CT_s\dot{T}^{\frac{c}{Ja_{HN}}} + T_s$$



Universal correlation vs. Experimental results

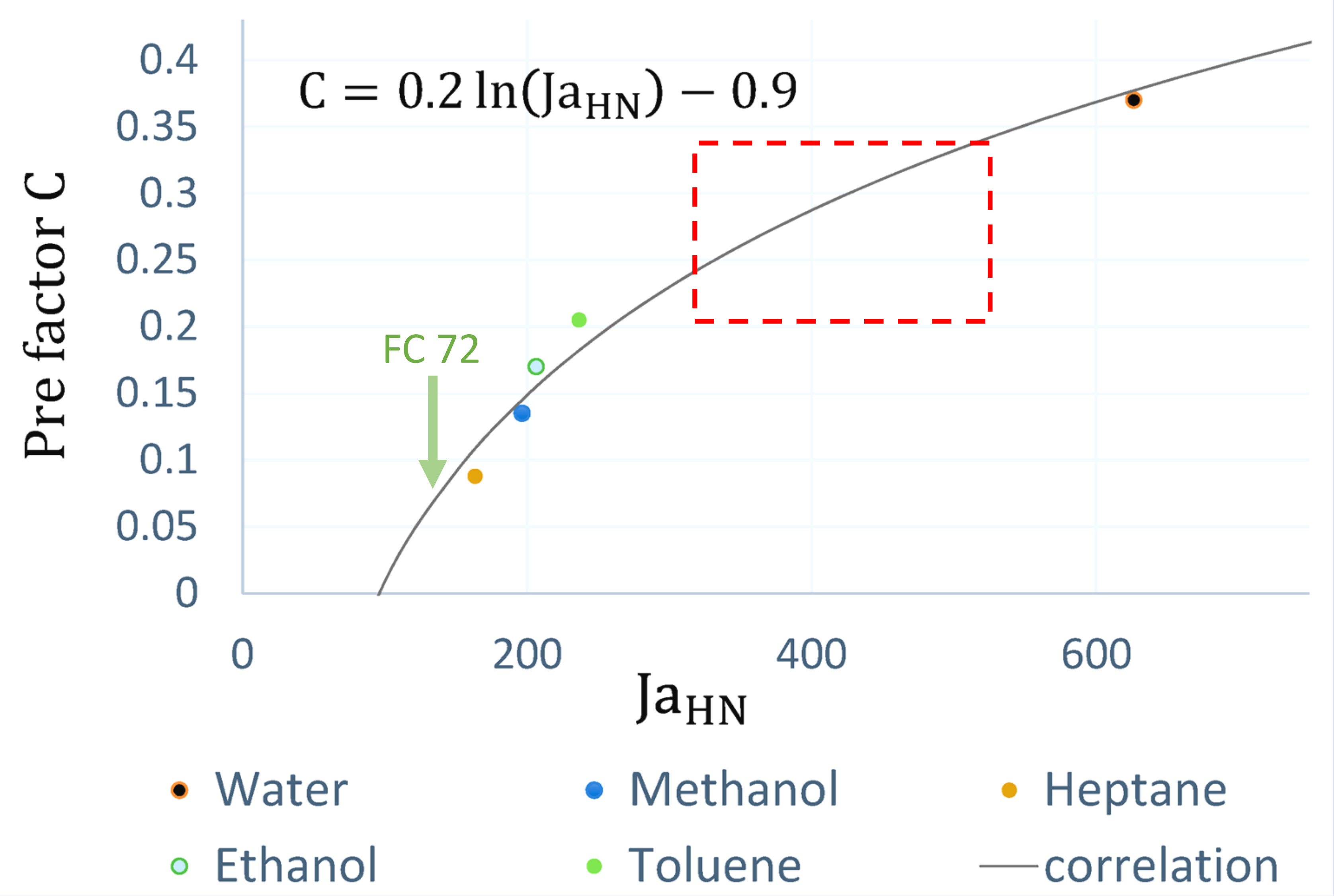


Ja_{HN}	Liquid	C	polar
626	Water	0.370	Y
196	Methanol	0.135	Y
206	Ethanol	0.170	N
136	Heptane	0.093	Y
236	Toluene	0.205	N

Bar-Kohany & Amsalem IJHMT, 2018

Universal Correlation - Pre factor C

Liquid	Pre factor C
Water	0.379
Methanol	0.136
Ethanol	0.169
Heptane	0.088
Toluene	0.200



Take home points

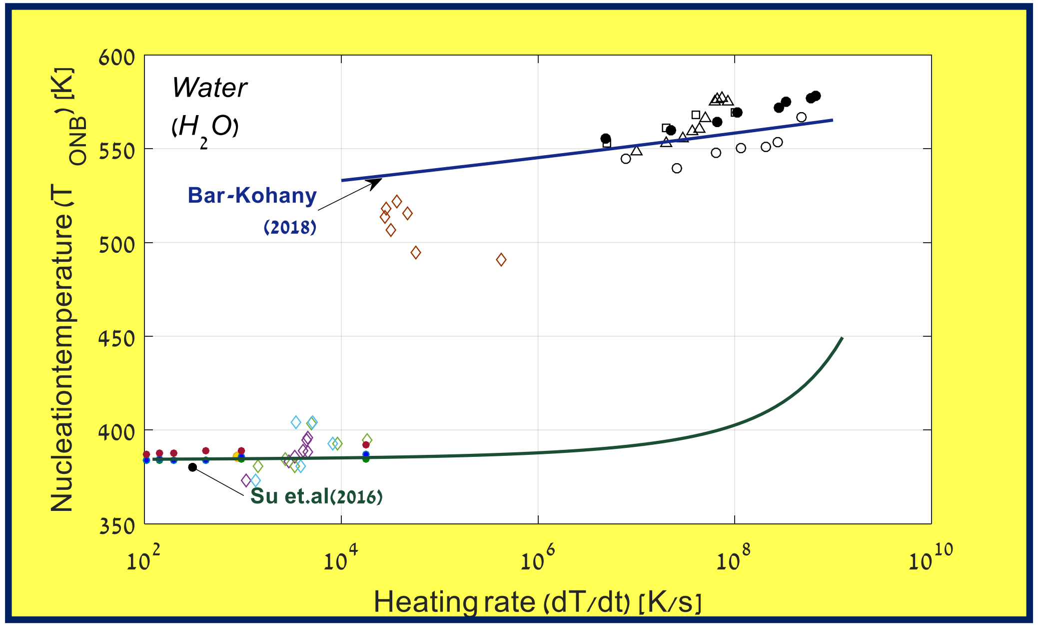
- A simple, universal correlation was developed to predict the T_{ONB} due to **rapid** isobaric process, as a function of the heating rate $(\dot{T})$.

$$\boxed{\Delta T_n = C\, T_s\, \dot{T}^{\frac{10}{Ja_{HN}}}}$$

- The input required is simply the ***saturation*** & ***HN*** conditions.
- The analysis considered **classical thermodynamic potentials** ***(Gb, Ja)*** and modified them to include **dynamic effects**.
- This correlation can be used in CFD codes

Future work

- Expanding the experimental data base:
  - Intermediate heating rates.
  - Different pressure values.
  - Different fluids. (C(Ja))
  - Flow boiling



- Formulation of a unifying model to predict slow → intermediate → fast processes.

- Same for rapid depressurization.

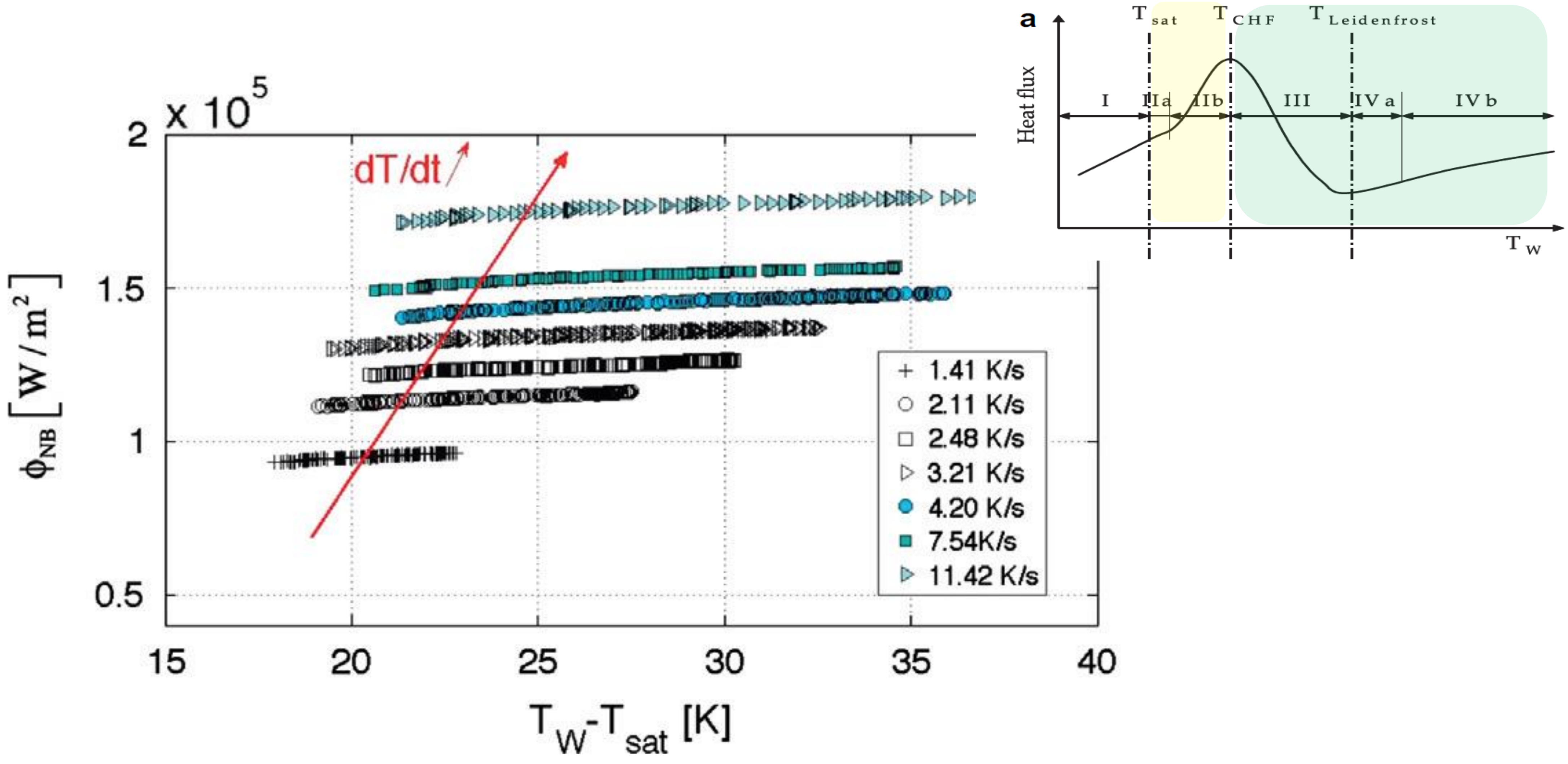
Any Questions ?

Yarden Amsalem

Wish to acknowledge the support of CHE-IAEC research grant by the PAZY Foundation.

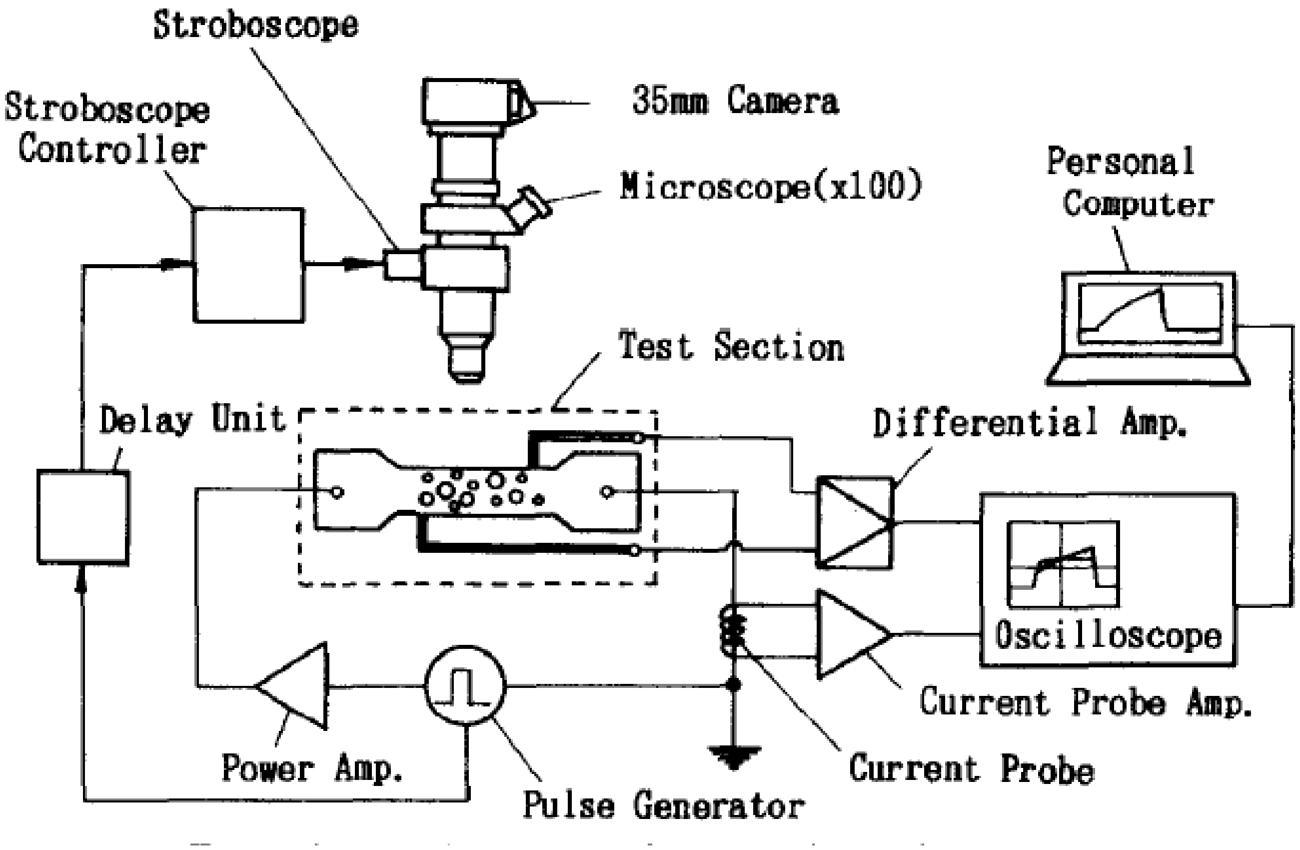
PAZY
EXCELLING IN SCIENCE

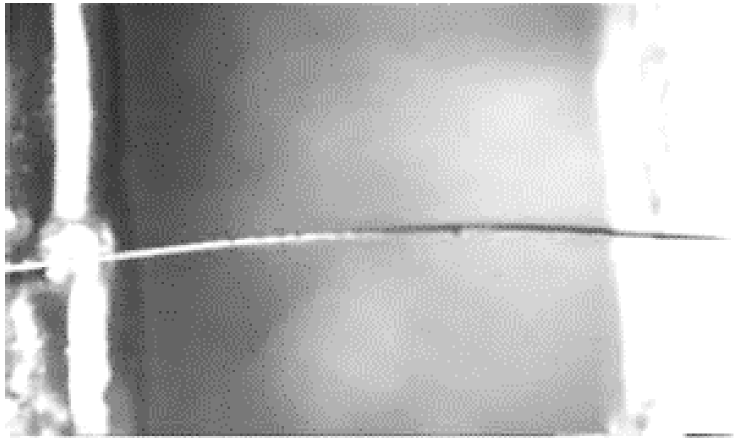
Fuel-drop impact onto heated, dry surfaces



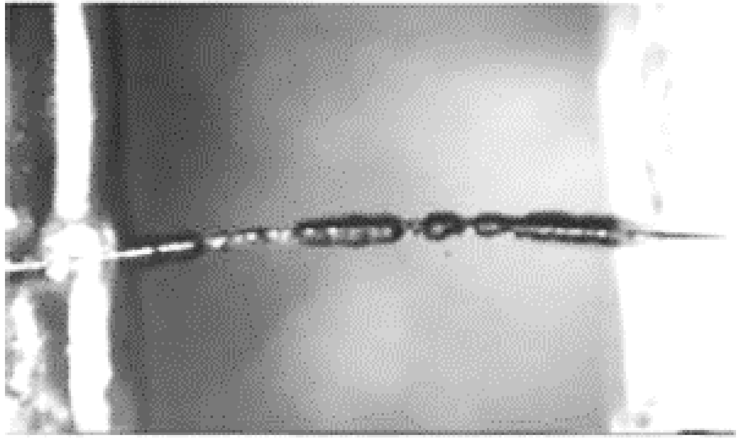
Visentini, Coiln & Ruyer, *Exp.Thermal.Fluid.Sci.* (2014)

Experimental Methods - Pulse Heating





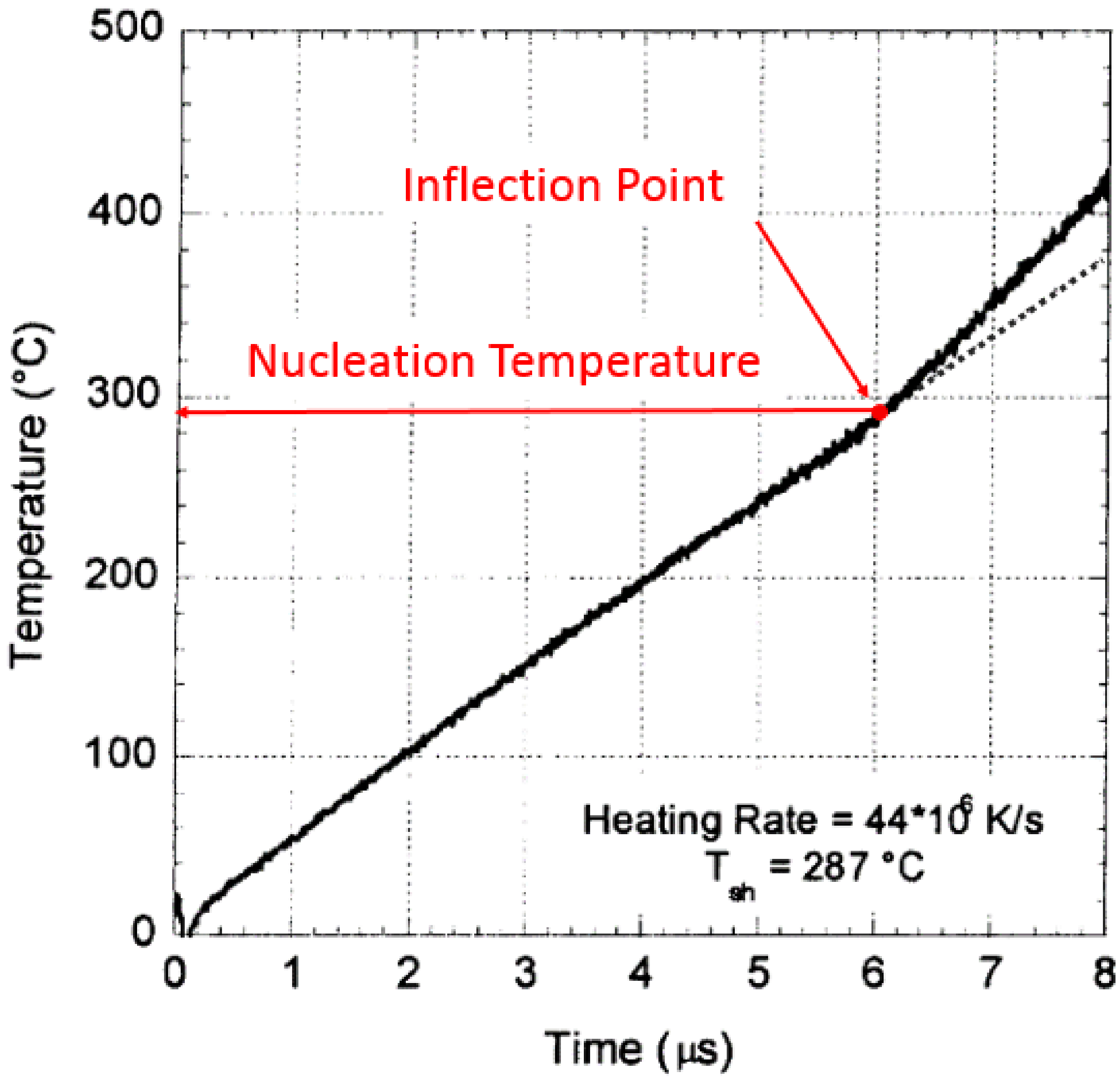
$\tau = 0$



$\tau = 17\mu s$

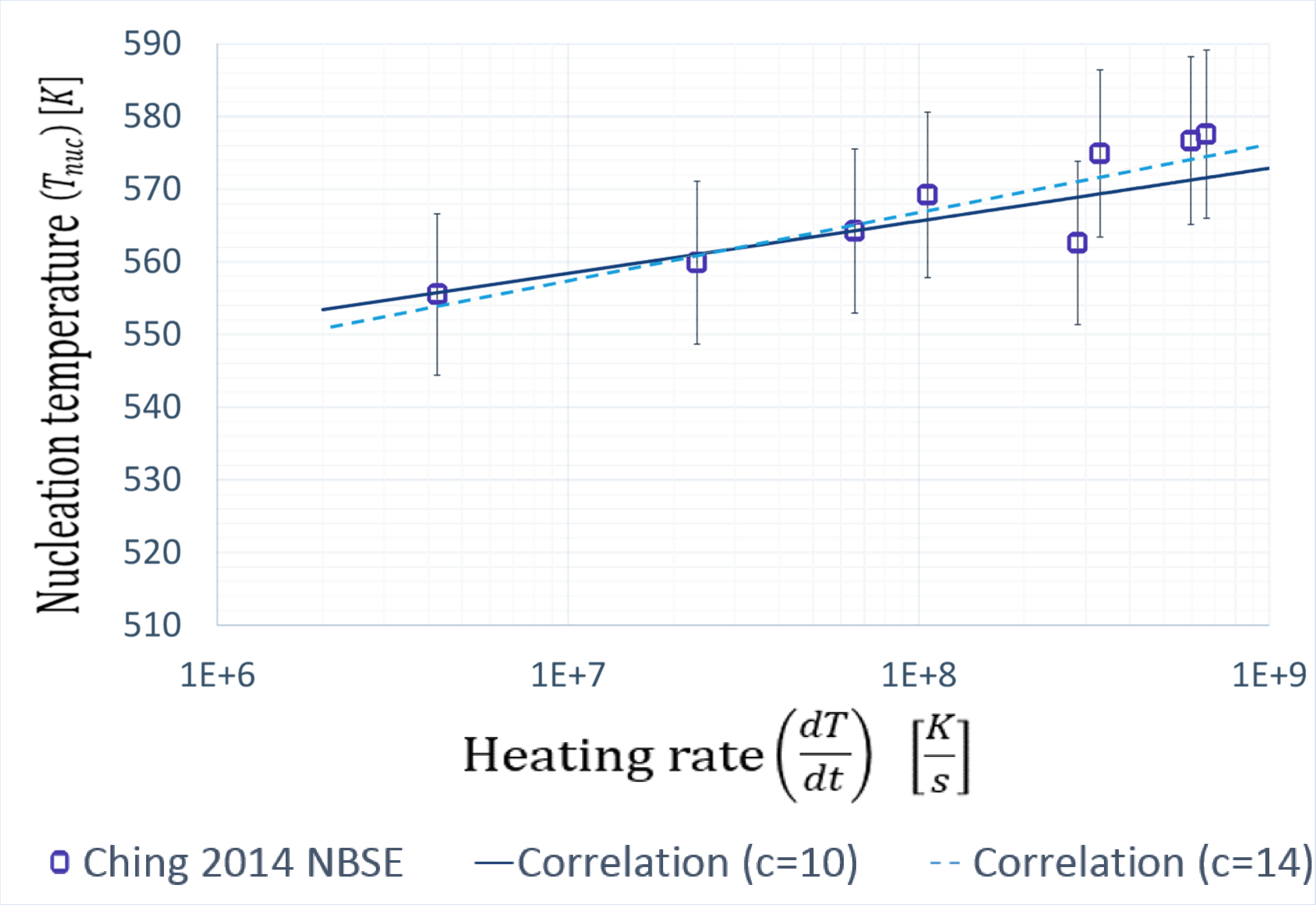
Y. Iida, K. Okuyama, K. Sakurai, Int. J. Heat Mass Transf. 1994

Experimental results



Glod .S., ;.D., Zhao .Z., Yadigaroglu .G, Int. J. Heat Mass Transf. 2002.

Universal Correlation - Factor c



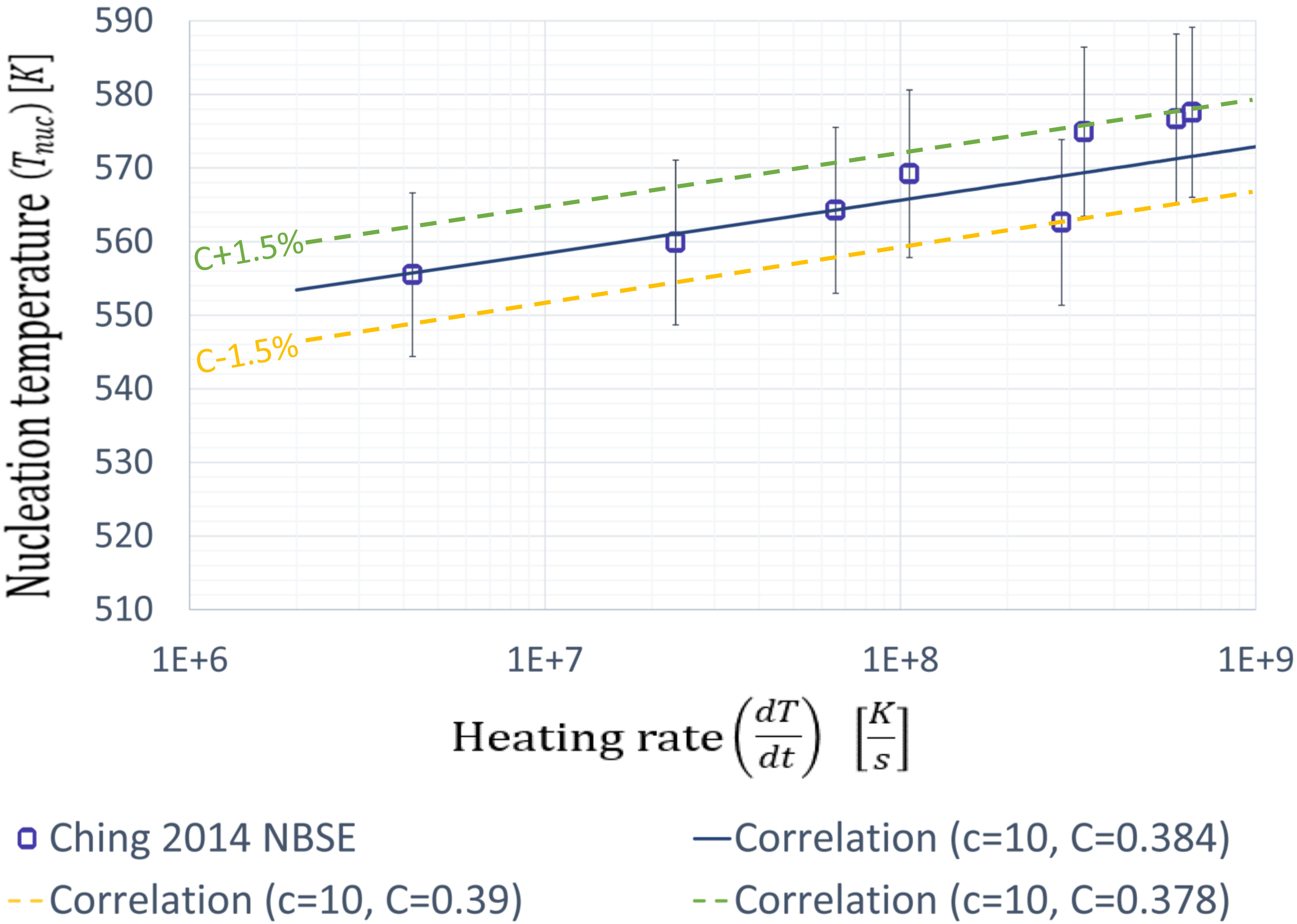
$$T_n \approx C T_s \dot{T}^{\frac{c}{Ja_{HN}}} + T_L$$

fitting factor c to each exp

fitting universal factor c

$$c \approx 10$$

Universal Correlation - Pre factor C



$$T_n \approx C T_s \dot{T}^{\frac{c}{Ja_{HN}}} + T_L$$

↓

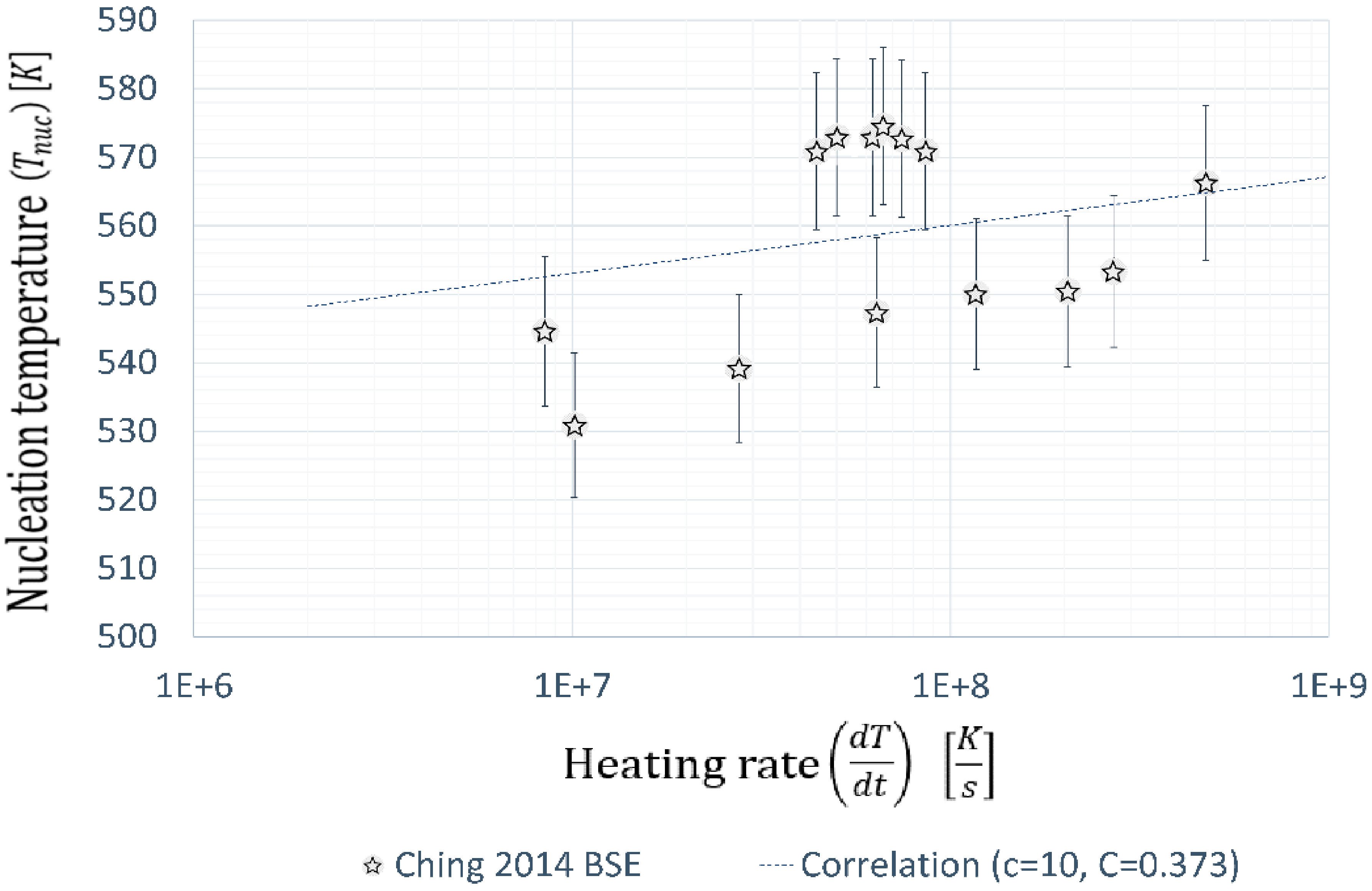
fitting pre factor C to each exp

↓

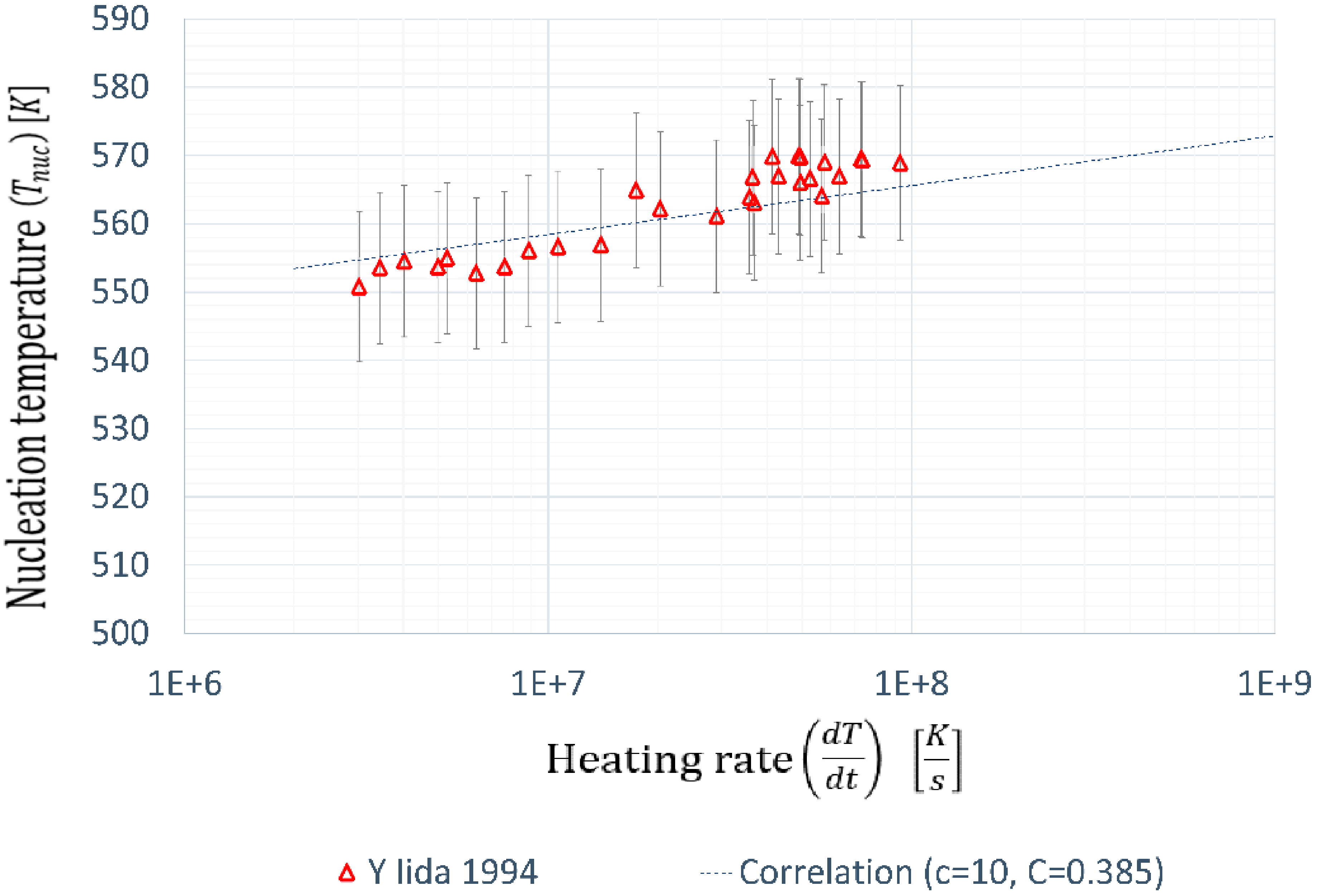
fitting universal pre factor C to each fluid

Universal Correlation - Pre factor C

Reference	C pre factor	Liquid
K. Okuyama 1994	0.385	Water
Thomas Avedisian 2014 BSE	0.373	
Thomas Avedisian 2014 NBSE	0.384	
S. Glod a, D. Poulikakos 2002	0.381	
Average value with tolerance	0.379±0.006	



Nucleation temperature (T_{nuc}) [K]
590
580
570
560
550
540
530
520
510
500
1E+6
1E+7
1E+8
1E+9
Heating rate $\left(\frac{dT}{dt}\right)$ $\left[\frac{K}{s}\right]$
☆ Ching 2014 BSE
Correlation (c=10, C=0.373)


Nucleation temperature (T_{nuc}) $[K]$
590
580
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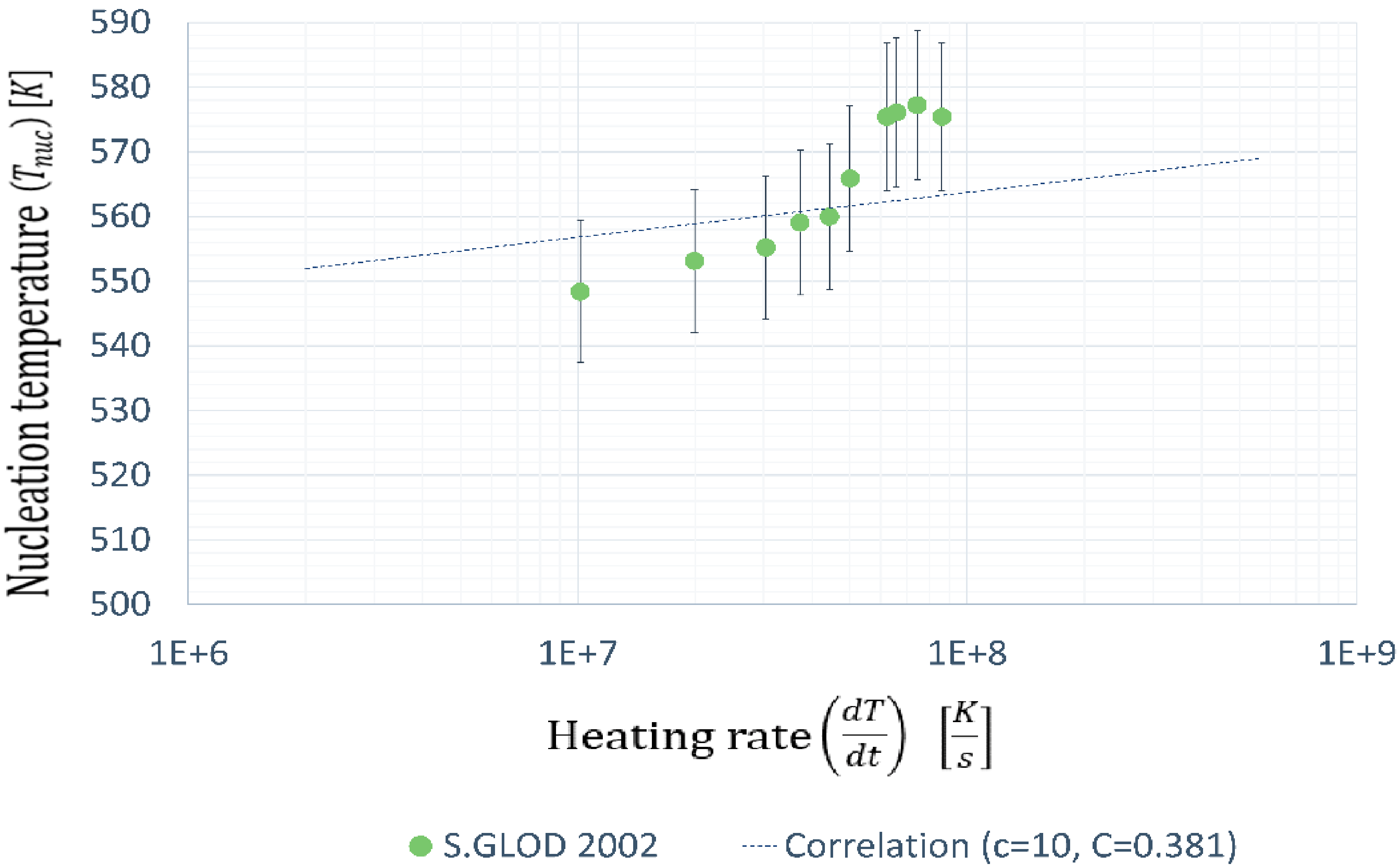
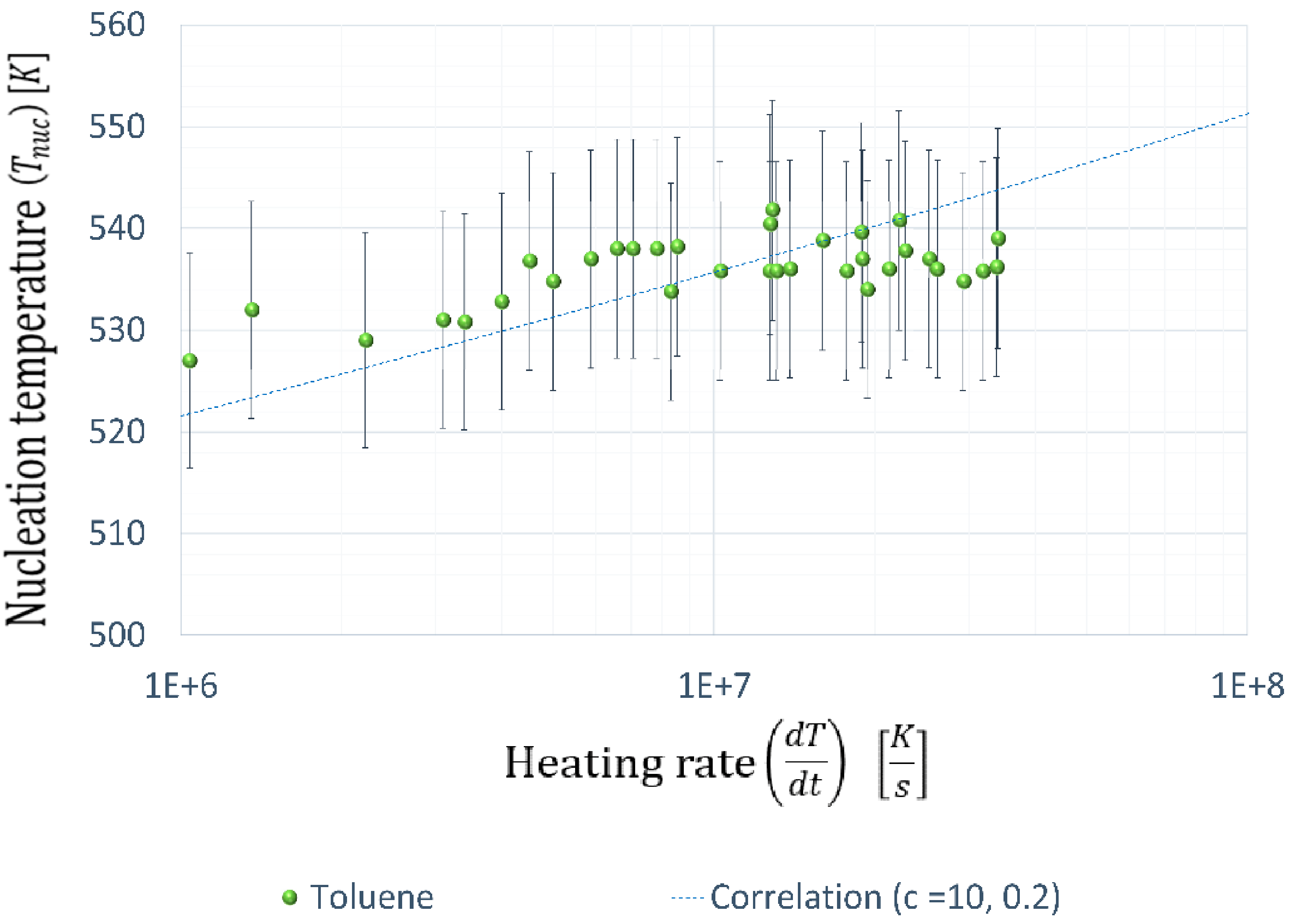
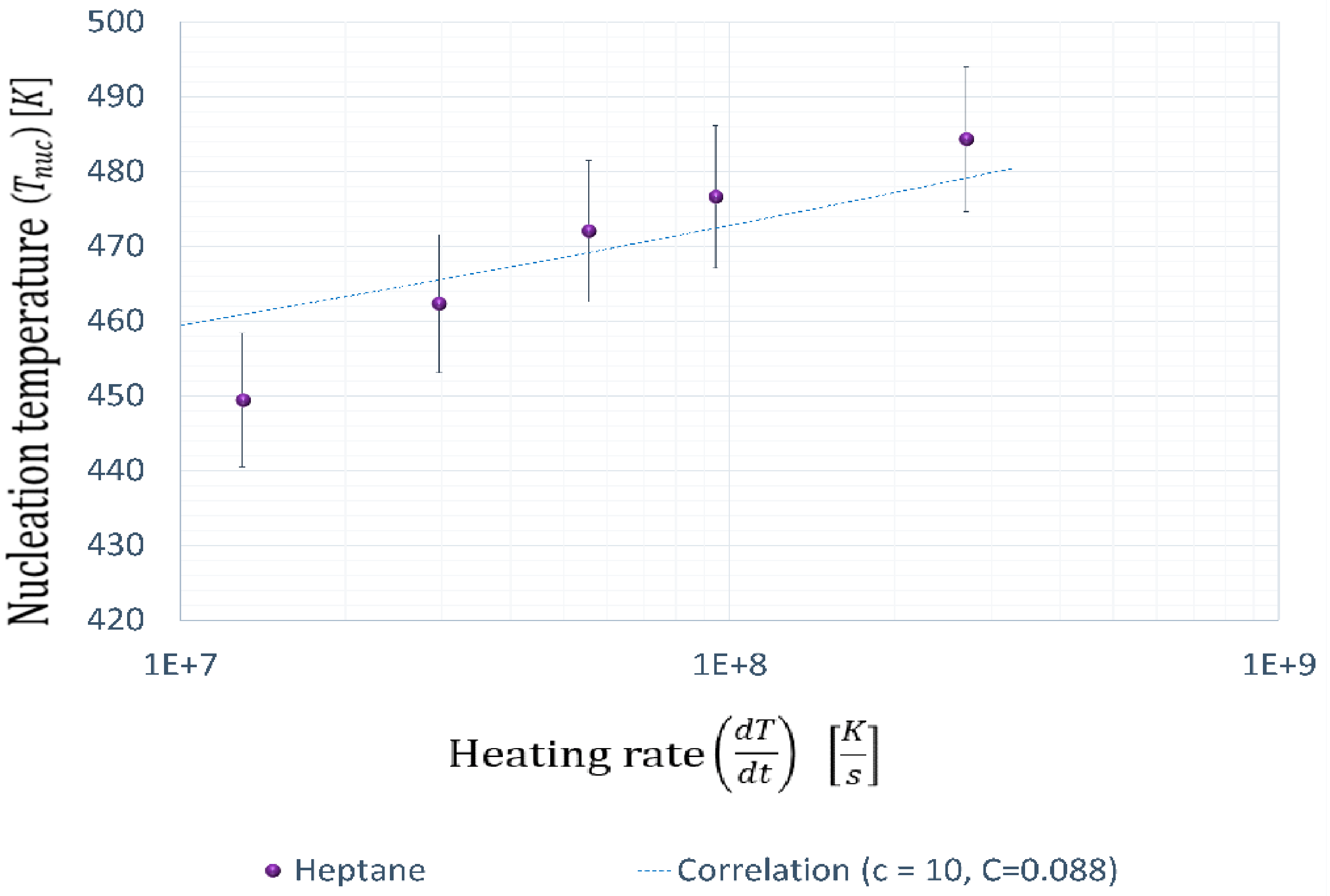
560
550
540
530
520
510
500
1E+6
1E+7
1E+8
1E+9
Heating rate $\left(\frac{dT}{dt}\right)$ $\left[\frac{K}{s}\right]$
Y Iida 1994
Correlation (c=10, C=0.385)

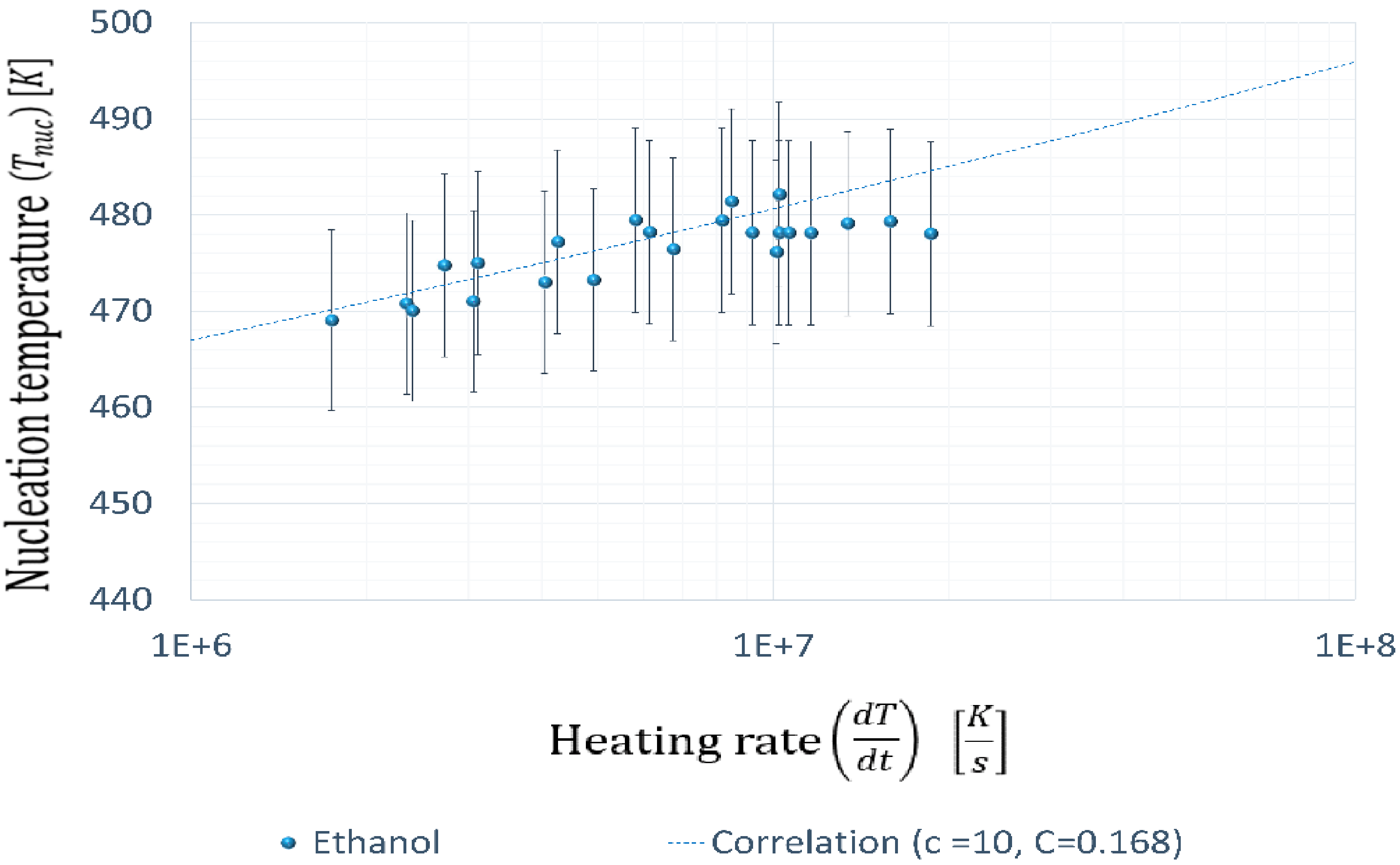


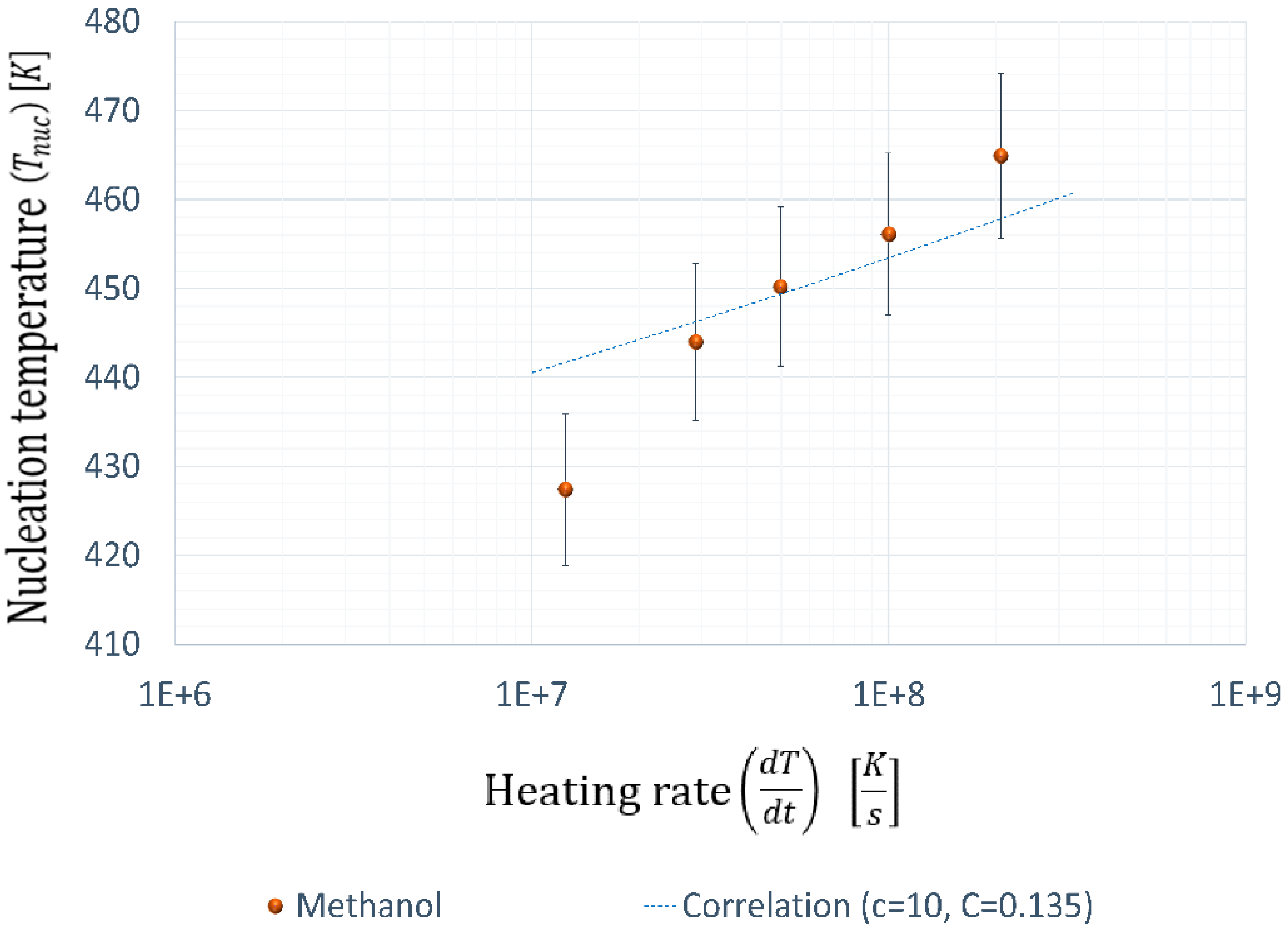
590
580
570
560
550
540
530
520
510
500
Nucleation temperature (T_{nuc}) $[K]$
1E+6
1E+7
1E+8
1E+9
Heating rate $\left(\frac{dT}{dt}\right)$ $\left[\frac{K}{s}\right]$
● S.GLOD 2002
Correlation (c=10, C=0.381)


560
550
540
530
520
510
500
Nucleation temperature (T_{nuc}) $[K]$
1E+6
1E+7
1E+8
Heating rate $\left(\frac{dT}{dt}\right)$ $\left[\frac{K}{s}\right]$
Toluene
Correlation (c =10, 0.2)

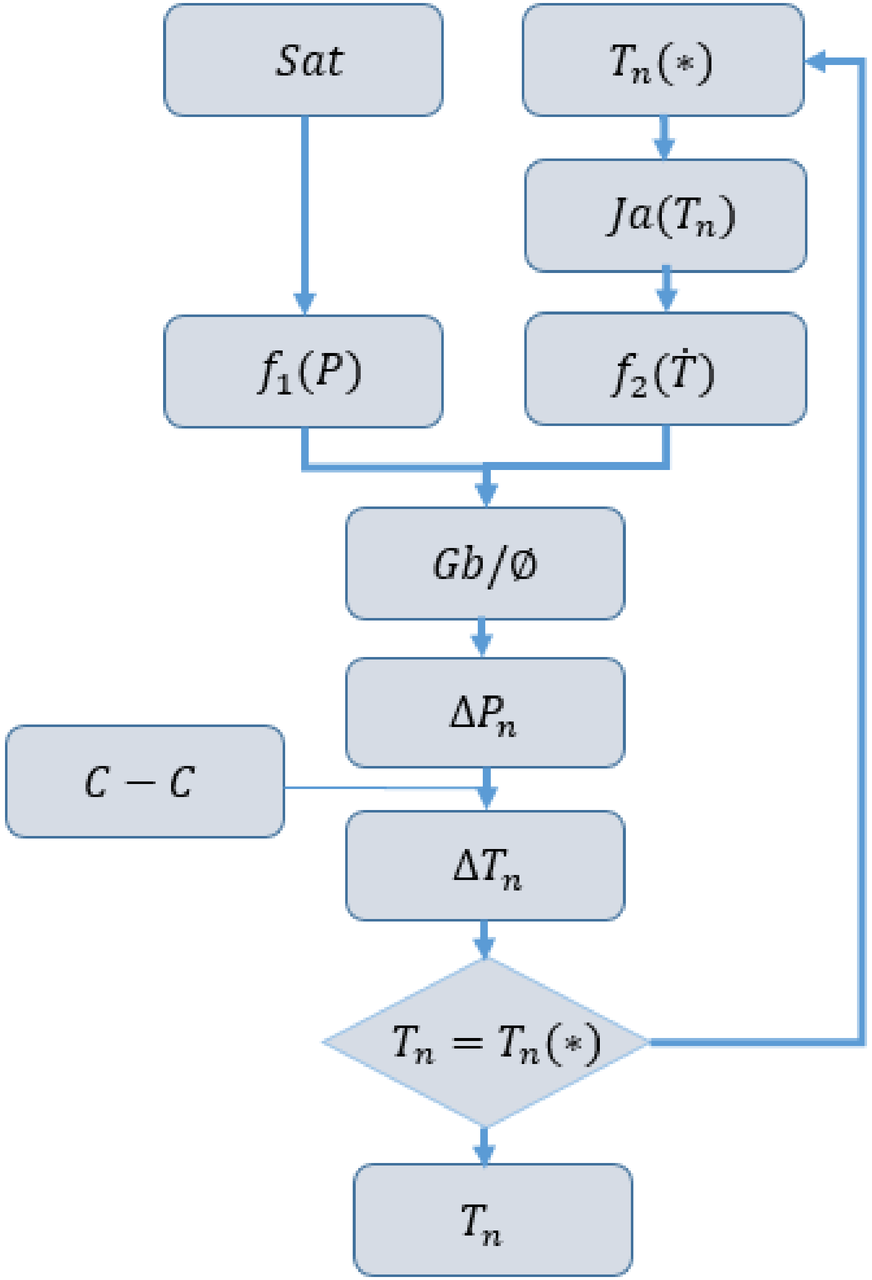


Nucleation temperature (T_{nuc}) $[K]$
500
490
480
470
460
450
440
430
420
1E+7
1E+8
1E+9
Heating rate $\left(\frac{dT}{dt}\right)$ $\left[\frac{K}{s}\right]$
Heptane
Correlation (c = 10, C=0.088)


500
490
480
470
460
450
440
Nucleation temperature (T_{nuc}) $[K]$
1E+6
1E+7
1E+8
Heating rate $\left(\frac{dT}{dt}\right)$ $\left[\frac{K}{s}\right]$
● Ethanol
Correlation (c =10, C=0.168)



480
470
460
450
440
430
420
410
Nucleation temperature (T_{nuc}) $[K]$
1E+6
1E+7
1E+8
1E+9
Heating rate $\left(\frac{dT}{dt}\right)$ $\left[\frac{K}{s}\right]$
● Methanol
Correlation (c=10, C=0.135)


Sat
$T_n(*)$
$Ja(T_n)$
$f_1(P)$
$f_2(\dot{T})$
$Gb/\emptyset$
ΔP_n
$C-C$
ΔT_n
$T_n = T_n(*)$
T_n