Uncertainty Quantification and Propagation in Multiphysics Modeling of the PVT Growth of the SiC Crystal

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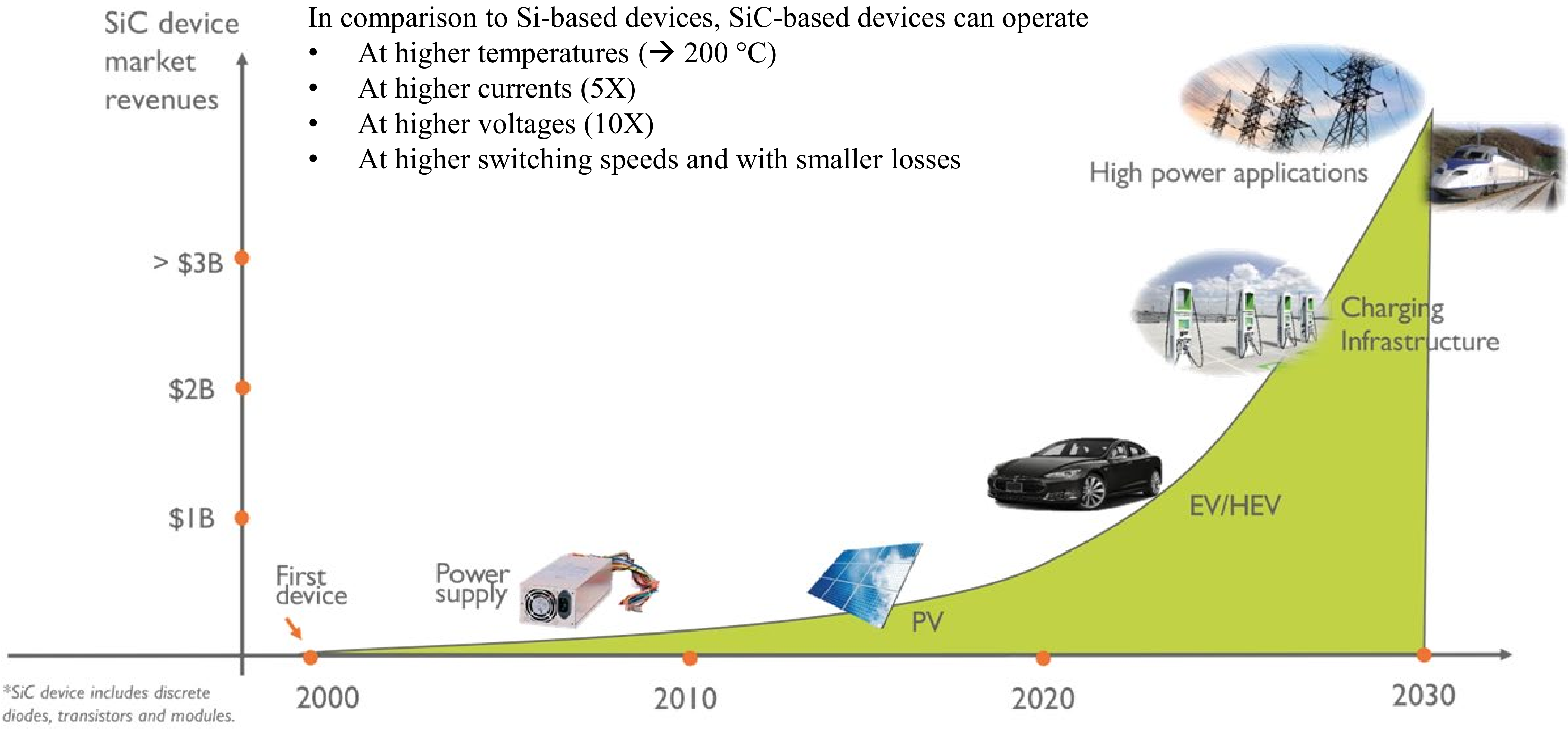
WHERE RESEARCH MEETS THE FUTURE

SiC in power electronics

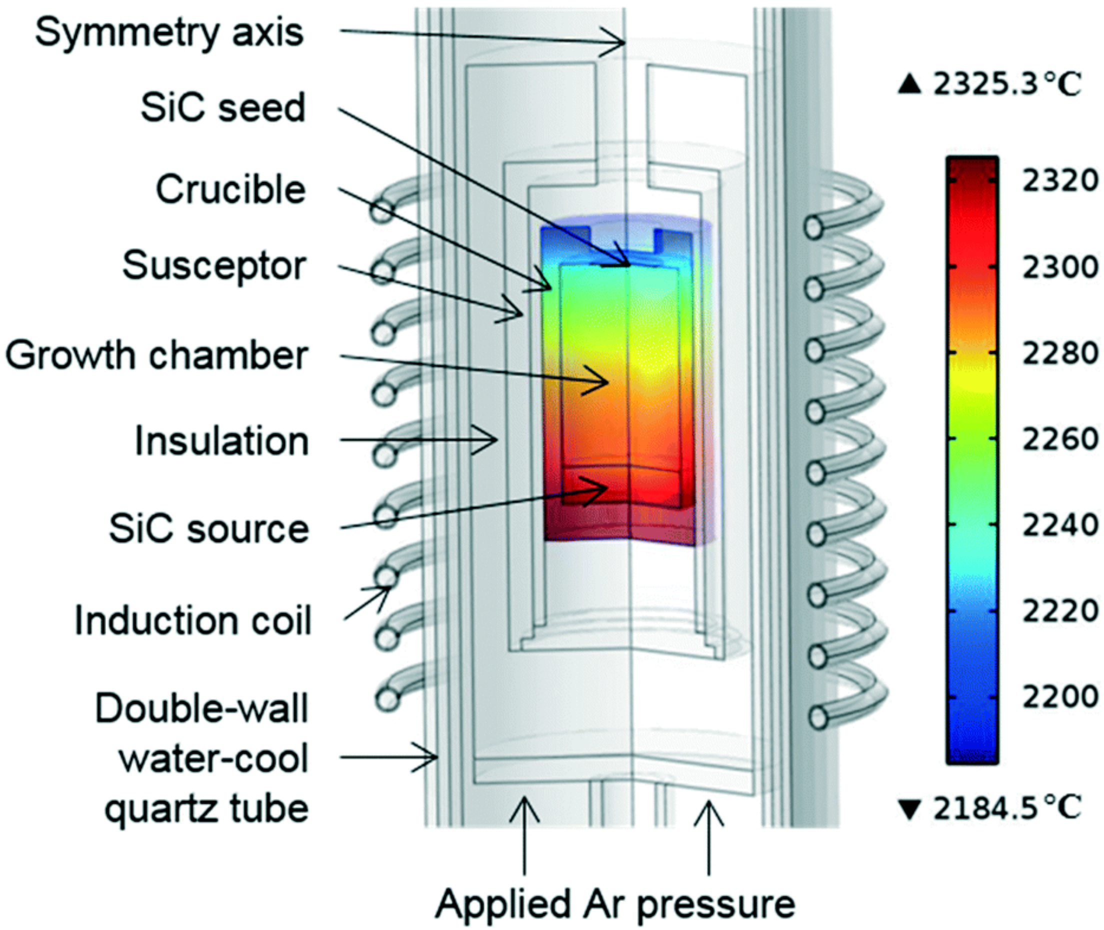
In comparison to Si-based devices, SiC-based devices can operate

- At higher temperatures (→ 200 °C)
- At higher currents (5X)
- At higher voltages (10X)
- At higher switching speeds and with smaller losses



Physical vapor transport (PVT)

- SiC single crystal growth via PVT involves inductive heating of the SiC source material to 2300 °C, causing SiC sublimation to various vapor species.
- These gas molecules condense on the cooler side, initiating crystal growth.
- Observing it externally is challenging.
- Simulation provides essential insights, including temperature distribution, mass transfer, gas composition, boule stresses, and crystal defects.



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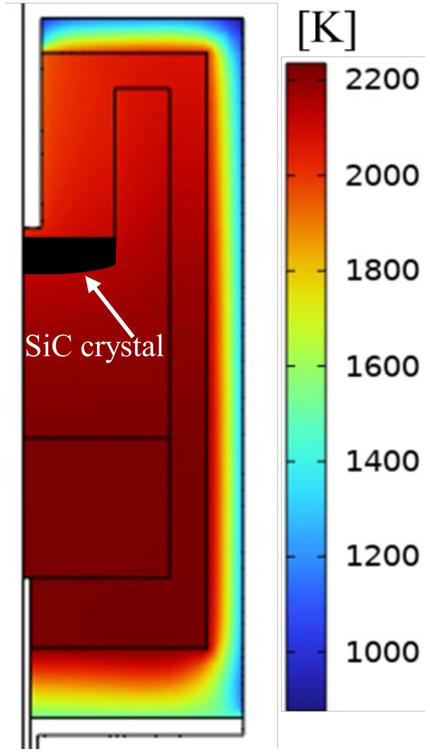
Motivation

➢ Temperature Control Significance :

- Precise temperature control at the seed surface is fundamental for growing high-quality SiC crystals.
- Temperature directly influences crystal quality, defect formation, and overall process efficiency.



➢ Uncertainty in Temperature Prediction:

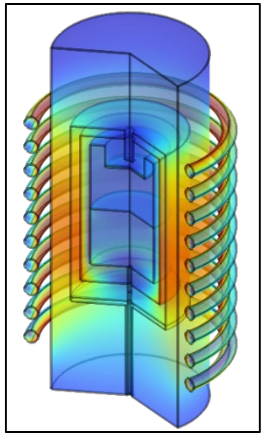
- Predicting temperature at the seed surface involves complex thermo-physical properties and models.
- Uncertainties in these properties and models can introduce variations in temperature forecasts.

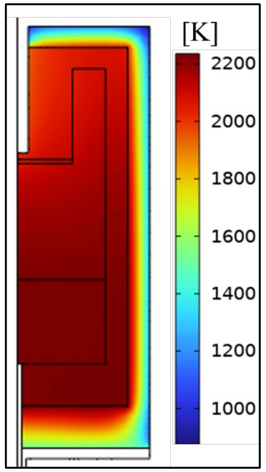
To account for the uncertainty in the thermo-physical material properties and various input parameters, a comprehensive uncertainty quantification and propagation analysis is needed.

Method

COMSOL multiphysics 6.1

- ❑ Electromagnetic heating
- ✓ AC/DC model
- ❑ Heat transfer
- ✓ Heat transfer in solids
- ✓ Surface to surface radiation : Ray shooting model
- ❑ Uncertainty quantification
- ✓ Screening
- ✓ Sensitivity analysis
- ✓ Uncertainty propagation





Uncertainty Quantification

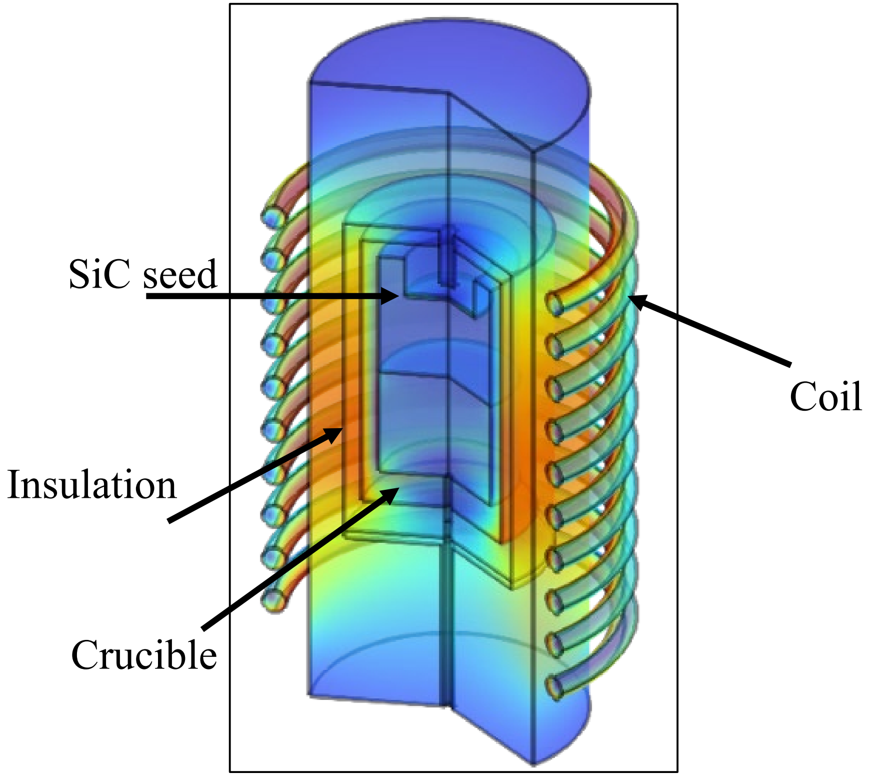
Input parameters

Parameter	Parameter range	Unit
Frequency	[6500-7500]	[Hz]
Coil power	[12.5-13.5]	[kW]
Electrical conductivity of insulation	[800-1200]	[S/m]
Coil position (r- direction)	[0.211-0.216]	[m]
Coil position (z-direction)	[0.005-0.015]	[m]
Emissivity of graphite (crucible)	[0.7-0.9]	[-]
Emissivity of SiC	[0.85-0.95]	[-]

Number of Input parameter: (m + 1)r
where r is the repetition number and m the number of input parameters.

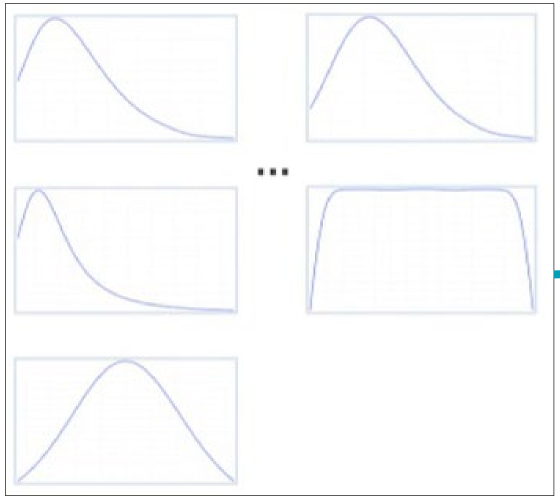
Quantity of interest (QoI)

Parameter	Unit
Seed average temperature	[degC]

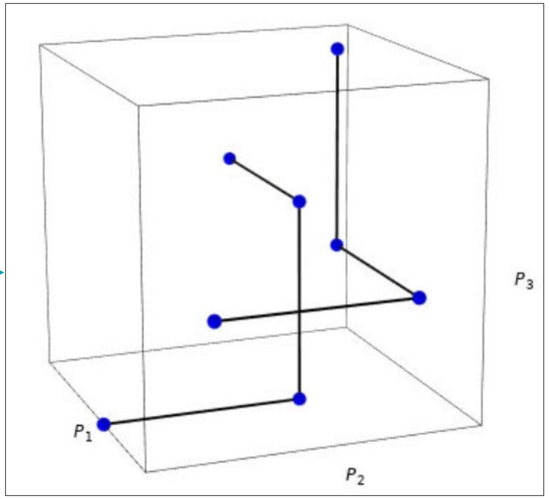


Uncertainty Quantification

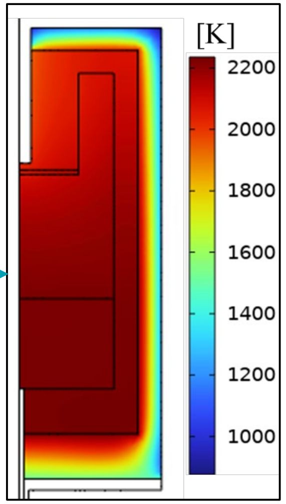
Screening, MOAT (Morris one-at-a-time method)



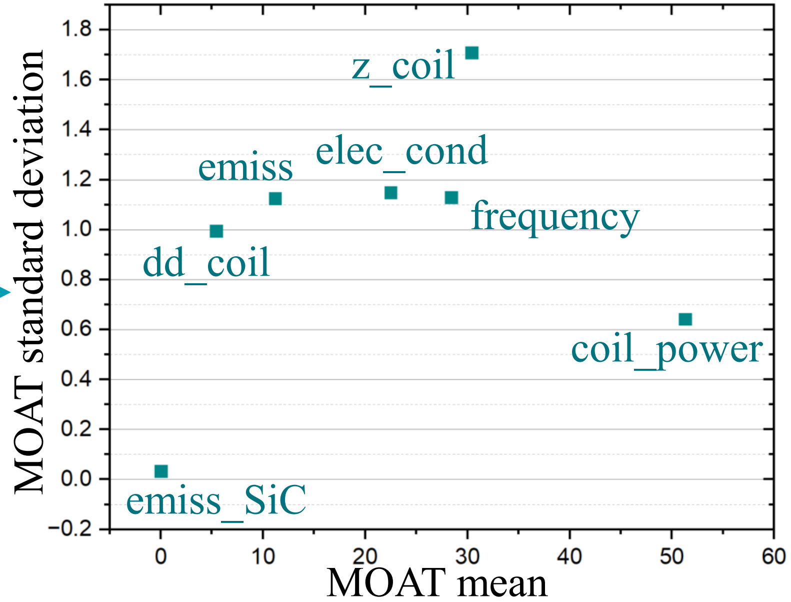
Input



Morris trajectories



Model evaluation



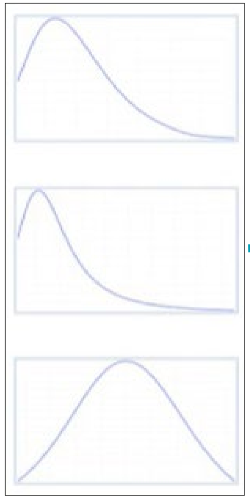
MOAT Results

MOAT mean for the i th input $\bar{\mu}_i = \frac{1}{r}\sum_{j=1}^{r} |d_{i,j}|$ where the elementary effect $d_{i,j} = \frac{f(\phi_{1,j}, \phi_{2,j}, \ldots, \phi_{i,j} \pm \Delta, \ldots, \phi_{m,j}) - f(\phi_{1,j}, \phi_{2,j}, \ldots, \phi_{m,j})}{\Delta}$

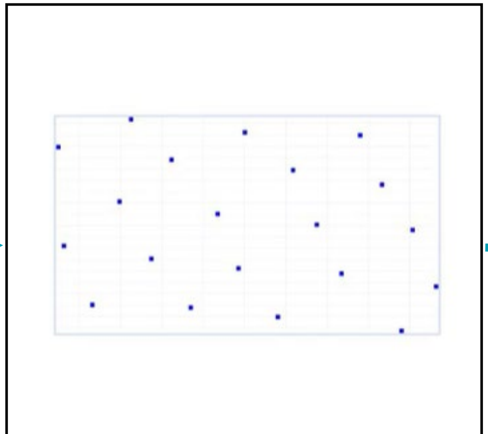
MOAT standard deviation for the i th input $\sigma_i = \sqrt{\frac{1}{r}\sum_{j=1}^{r} (d_{i,j} - \mu_i)^2},$

Uncertainty Quantification

Sensitivity analysis and uncertainty propagation



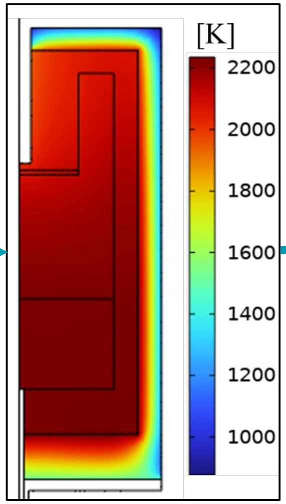
Input



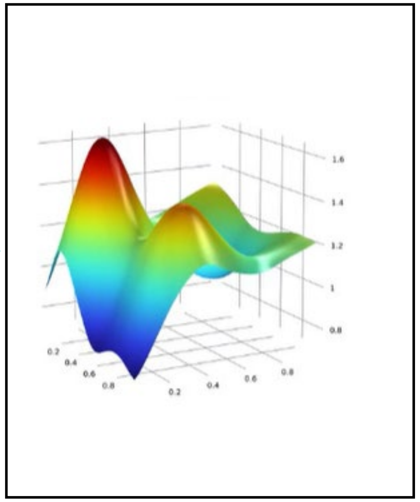
N~ 20n

Design of experiment

Latin hypercube
n number of the inputs, N is the number of model evaluations



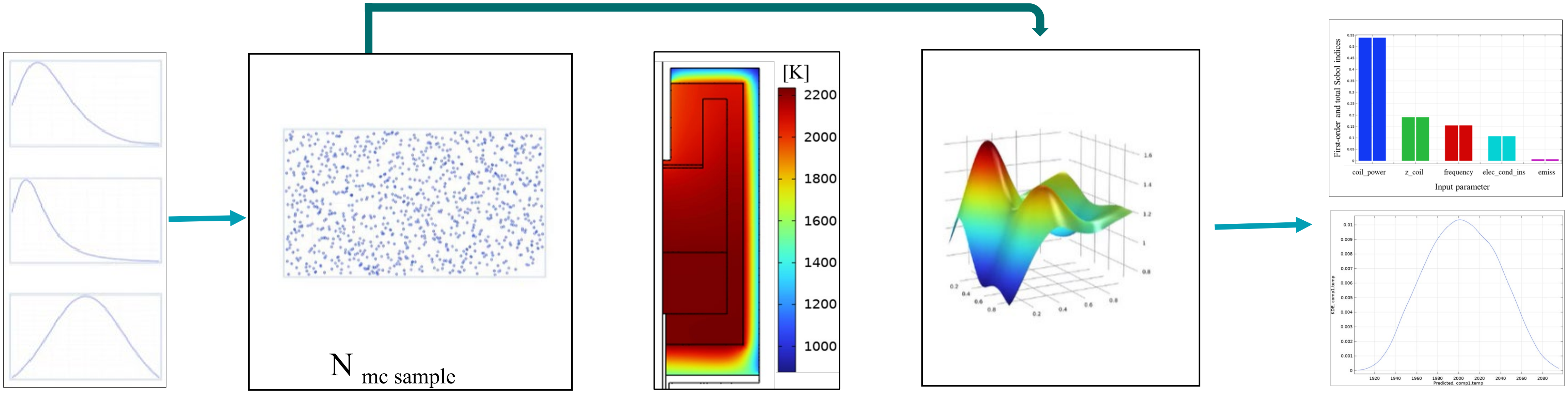
Model evaluation



Surrogate model

Uncertainty Quantification

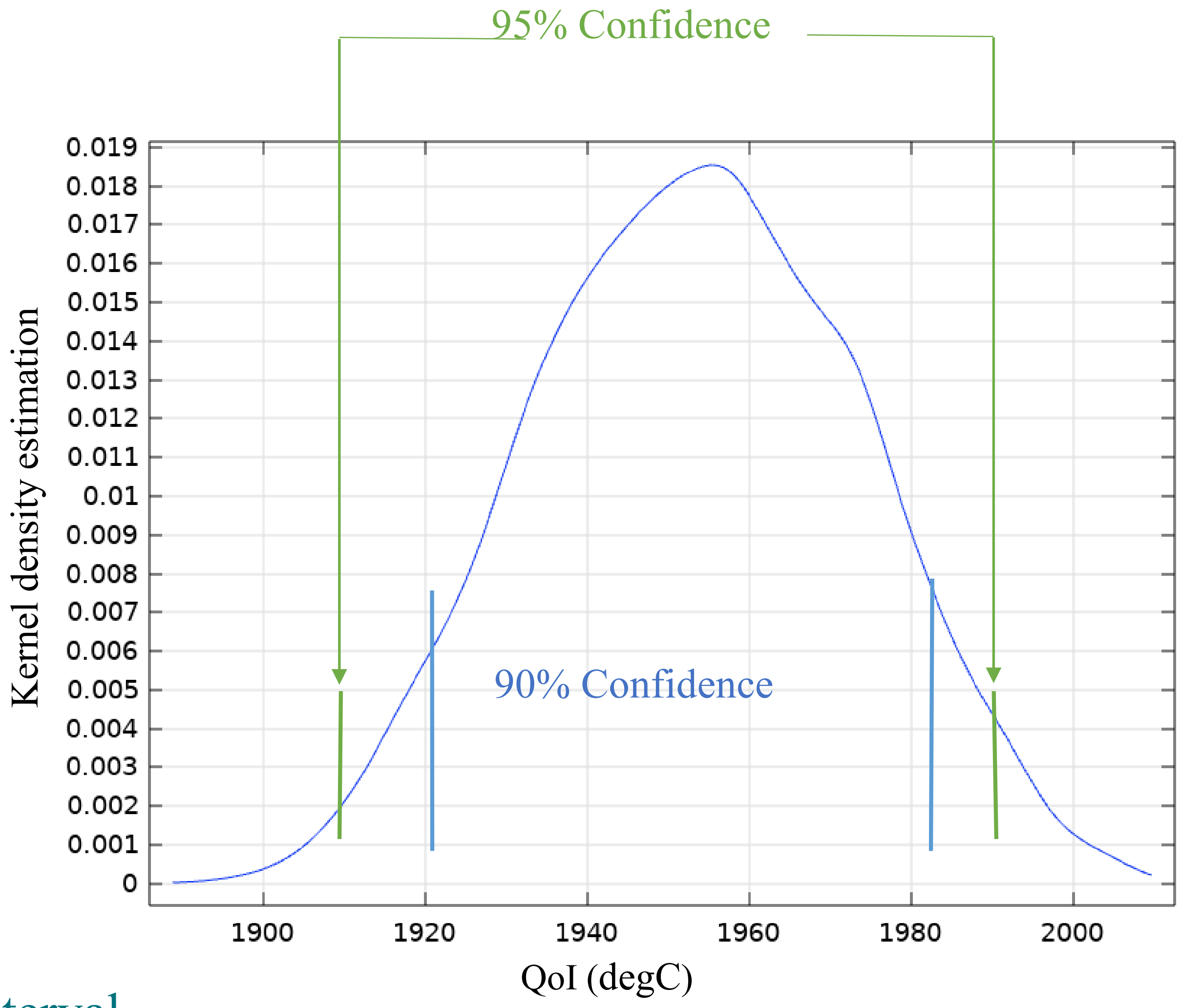
Sensitivity analysis and uncertainty propagation



Input | Design of experiment | Model evaluation | Surrogate model | UQ results

Uncertainty Quantification

Uncertainty propagation



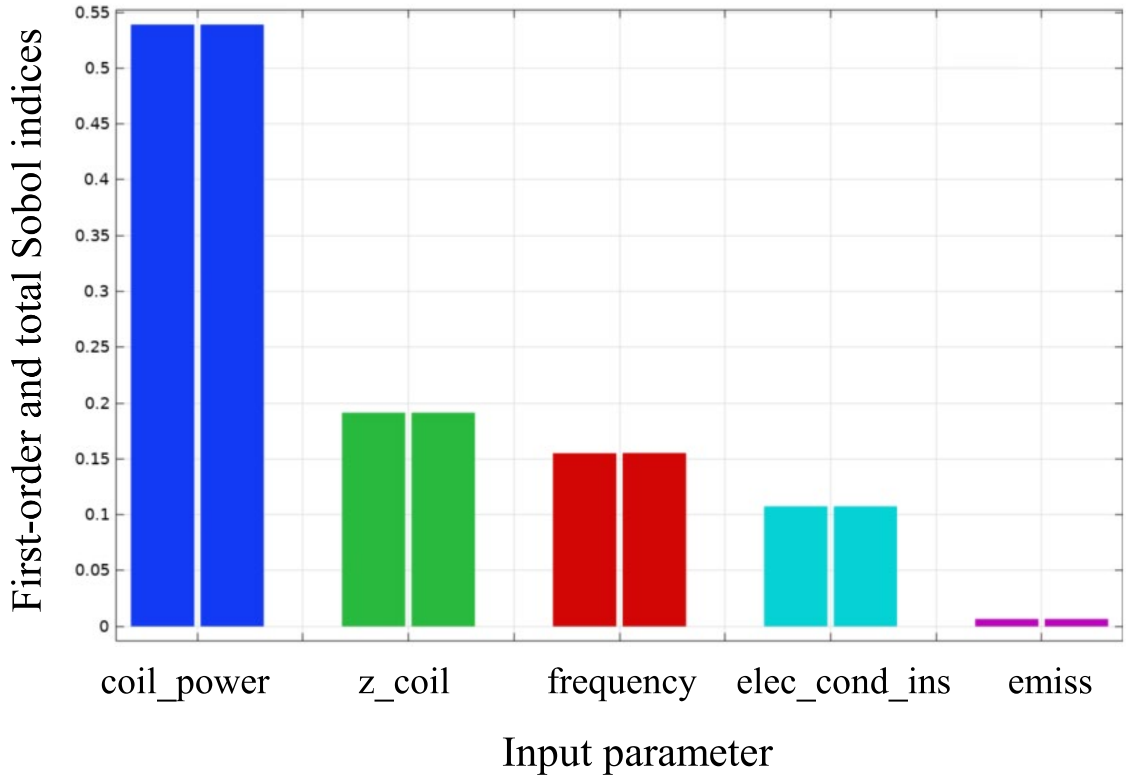
QoI confidence interval

	Mean	STD	Min	Max	Lower 90%	Upper 90%	Lower 95%	Upper 95%	Lower 99%	Upper 99%
QoI(degC)	1953.43	20.016	1888.2	2009.6	1920.2	1986.3	1915.2	1991.17	1905.8	2001.5

Uncertainty Quantification

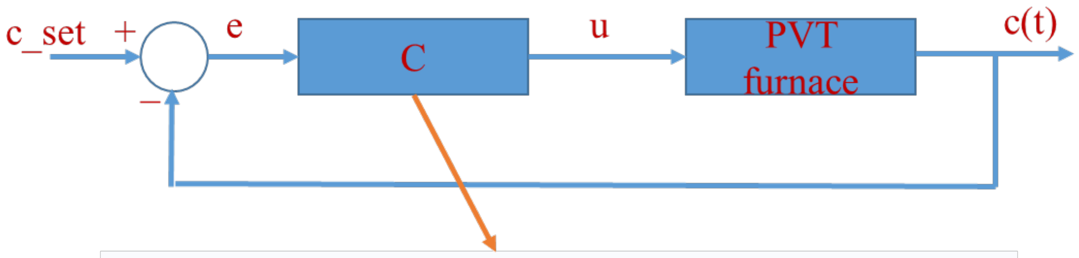
Sensitivity analysis

- Sobol indices (variance decomposition method, analysis of variance (ANOVA)).
- The primary goal of Sobol indices is to quantify and rank the sensitivity of a QoI to input parameters.
- Sobol indices break down the variance of the model's output into contributions from individual parameters and their interactions.

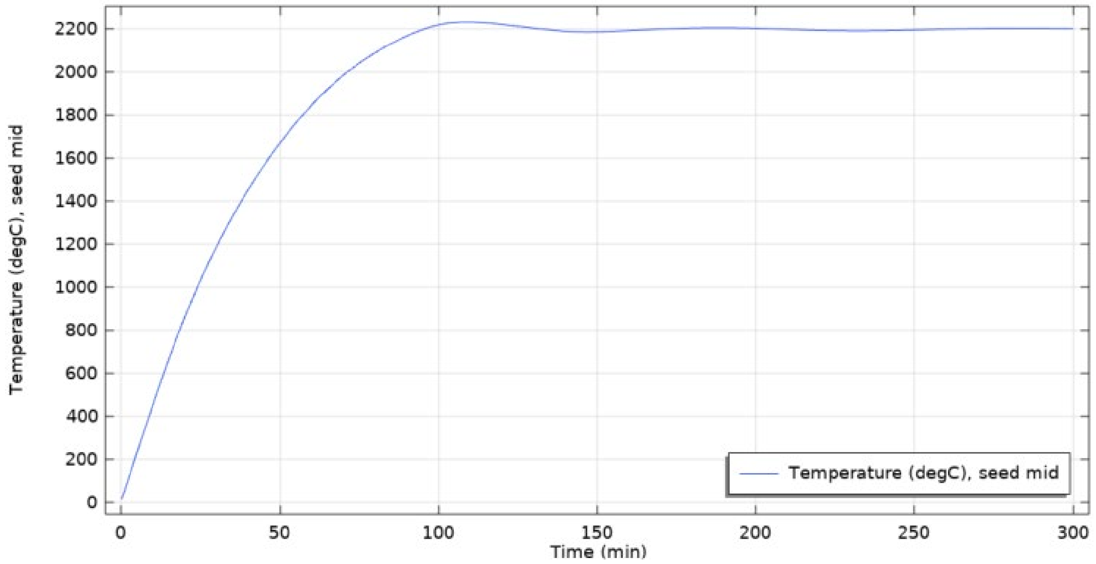


Controlling temperature in the furnace

Proportional-Integral-Derivative (PID)



$$u(t) = u_{\text{bias}} + k_{\text{p}}[c_{\text{set}} - c(t)] + k_{\text{i}}\int_0^t [c_{\text{set}} - c(\tau)]\,d\tau - k_{\text{d}}\frac{d}{dt}c(t)$$



Conclusion

- Numerical modeling provide a further understanding of the physicochemical behaviors of the crystal growth system and accelerate process optimization for SiC bulk crystal growth.

- Due to the uncertainty of the thermo-physical material properties and various input parameters, a thorough uncertainty quantification and propagation analysis is conducted.

- Uncertainty quantification highlights that power, frequency, and the position of the coils along the z-axis significantly impact the temperature of the seed surface.

Thank you for your attention!

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