Transient 2D modelling of Czochralski crystal growth process

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EIROPAS REĢIONĀLĀS ATTĪSTĪBAS FONDS
EIROPAS SAVIENĪBA
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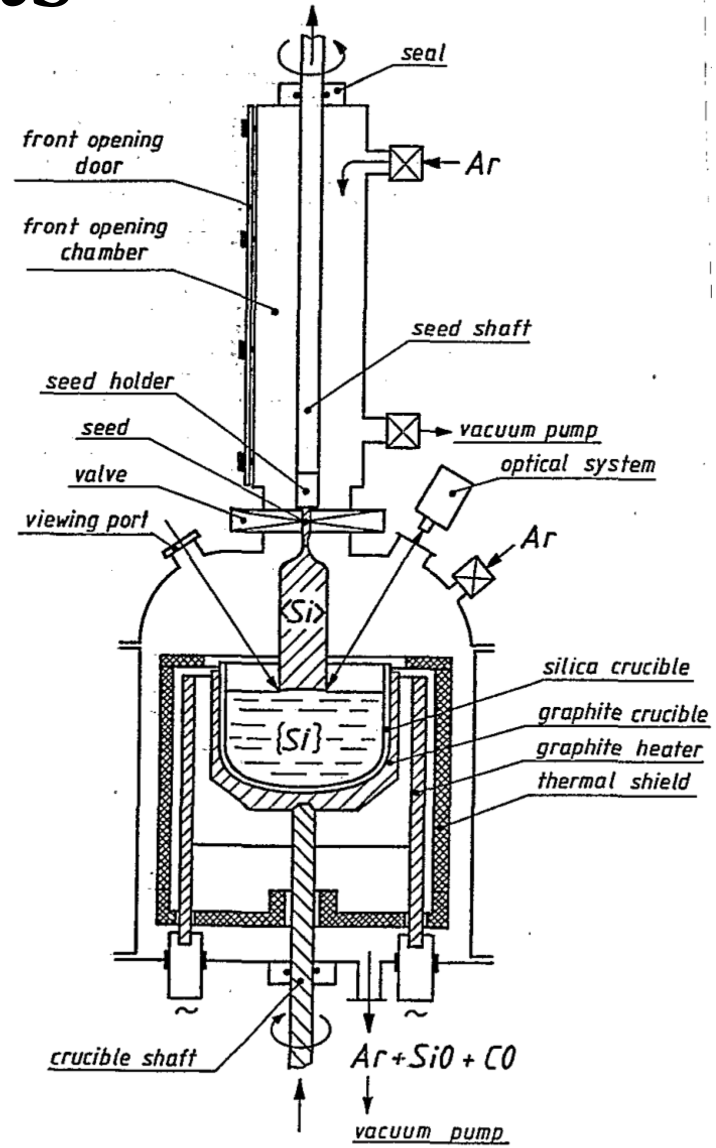


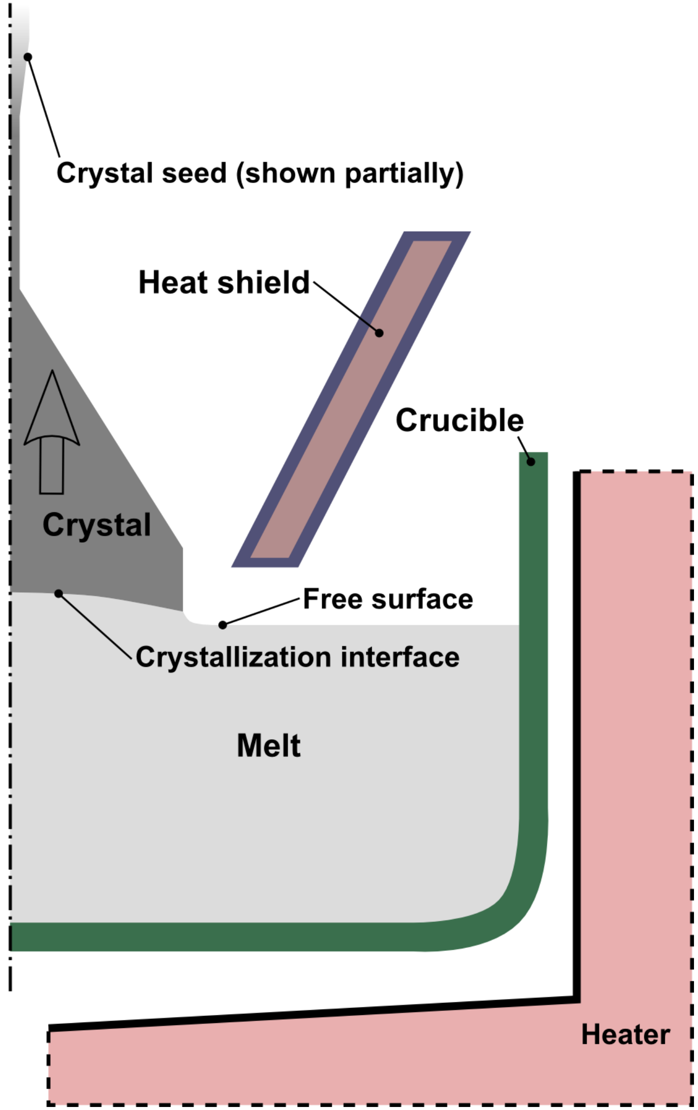
W. Zulehner. Mater. Sci. Eng. B, 73(1):7-15, 2000

Introduction

Czochralski (CZ) method for crystal growth

- Crystal diameter and growth rate has to be controlled in a certain range, which is achieved by process control

- The conventional control scheme consists of two PID controllers, which adjust crystal pulling velocity and heater power



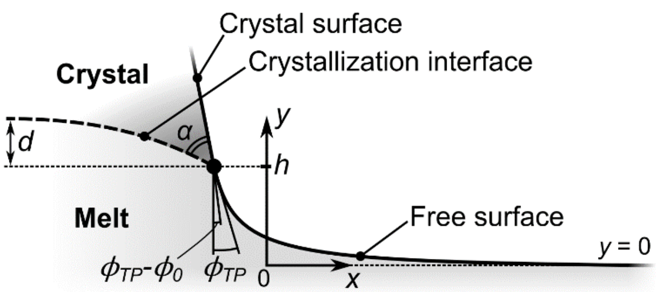
Introduction

Non-stationarity of CZ process

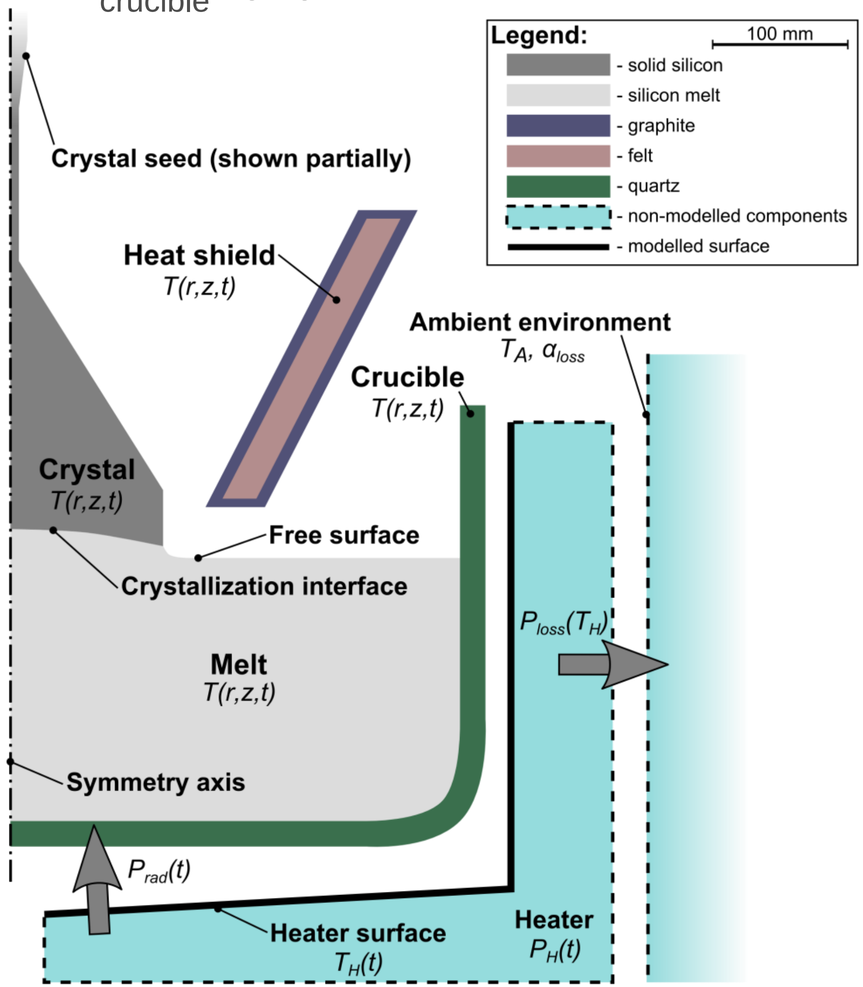
- The entire crystal growth process is highly non-stationary
- Effective mathematical and numerical methods are therefore needed
- Our model is
  - axisymmetric and with a simplified heater description (computationally inexpensive yet realistic)
  - fully transient with moving crystal and crucible and implemented PID control
  - with focus on the triple point region and crystal shape formation (triple point and shape are NOT fixed)

Mathematical model

- Non-stationary temperature field in crystal, melt, crucible, heat shield
- A simplified integral model for heater
- Hydrostatic approximation for meniscus shape
- Time-varying shape of crystallization interface, crystal length and radius

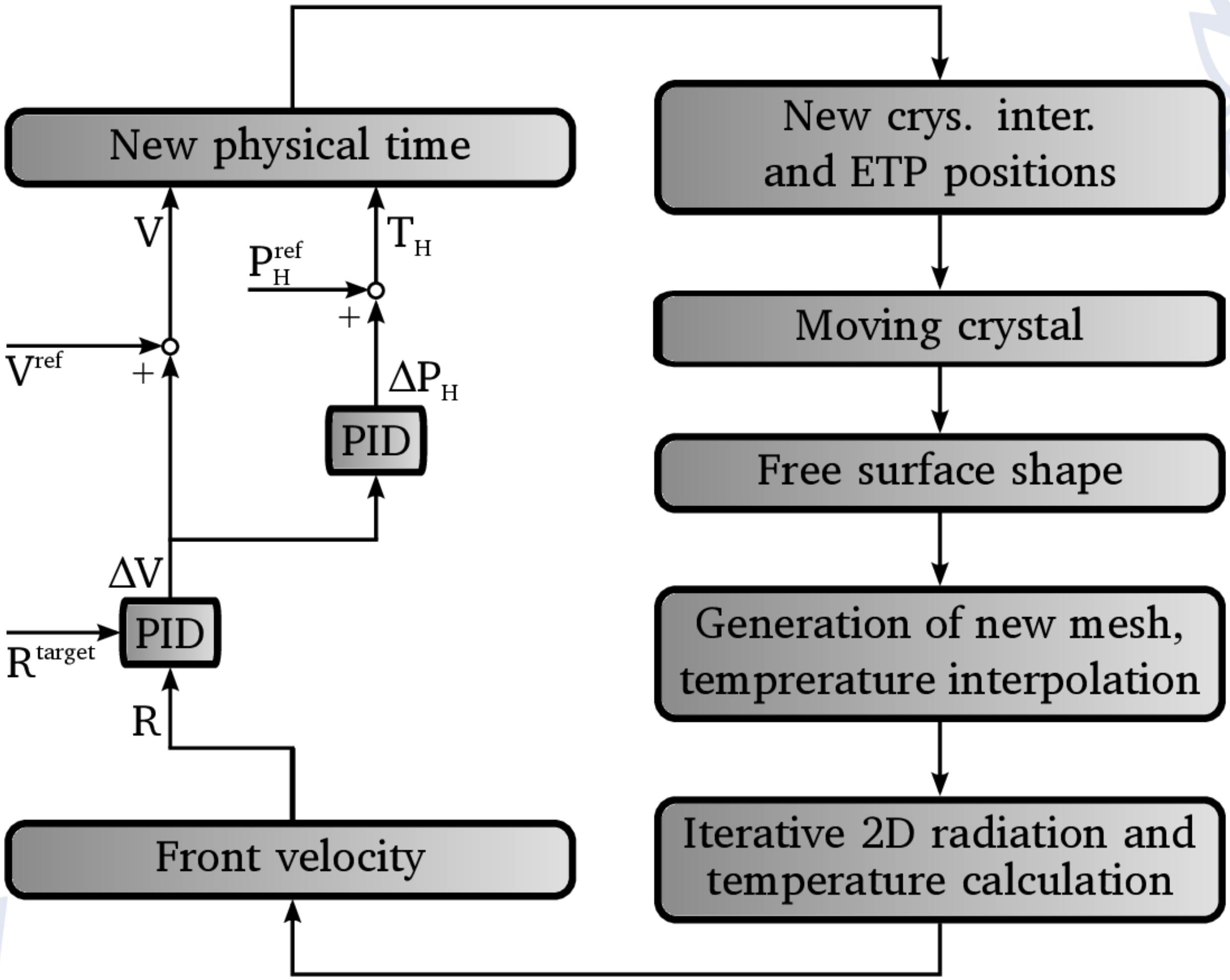


$D_{crystal}$=200 mm
$D_{crucible}$=640 mm



Mathematical model

Simulation algorithm



(growing)

(and crucible)

(adapting)

(radiation > temperature> radiation)

Calculation example

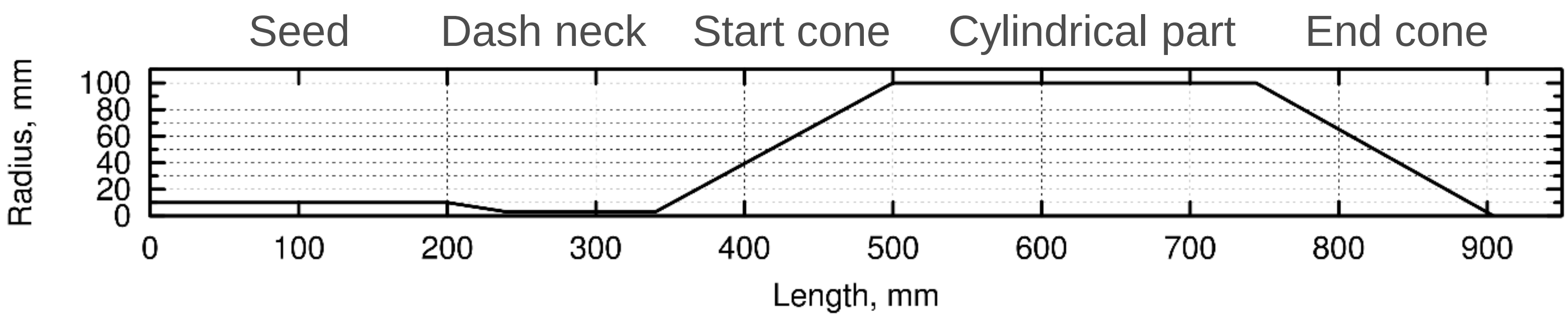
Introduction

- Calculations have been carried out for full CZ process (all growth stages)
  - seeding and Dash neck
  - start cone
  - cylindrical part
  - end cone
- This is important because optimal heater settings (power curve) can be predicted only when the whole CZ process is modelled. Due to thermal inertia, each process step cannot be considered separately

Calculation example

Process control

- The crystal radius setpoint:

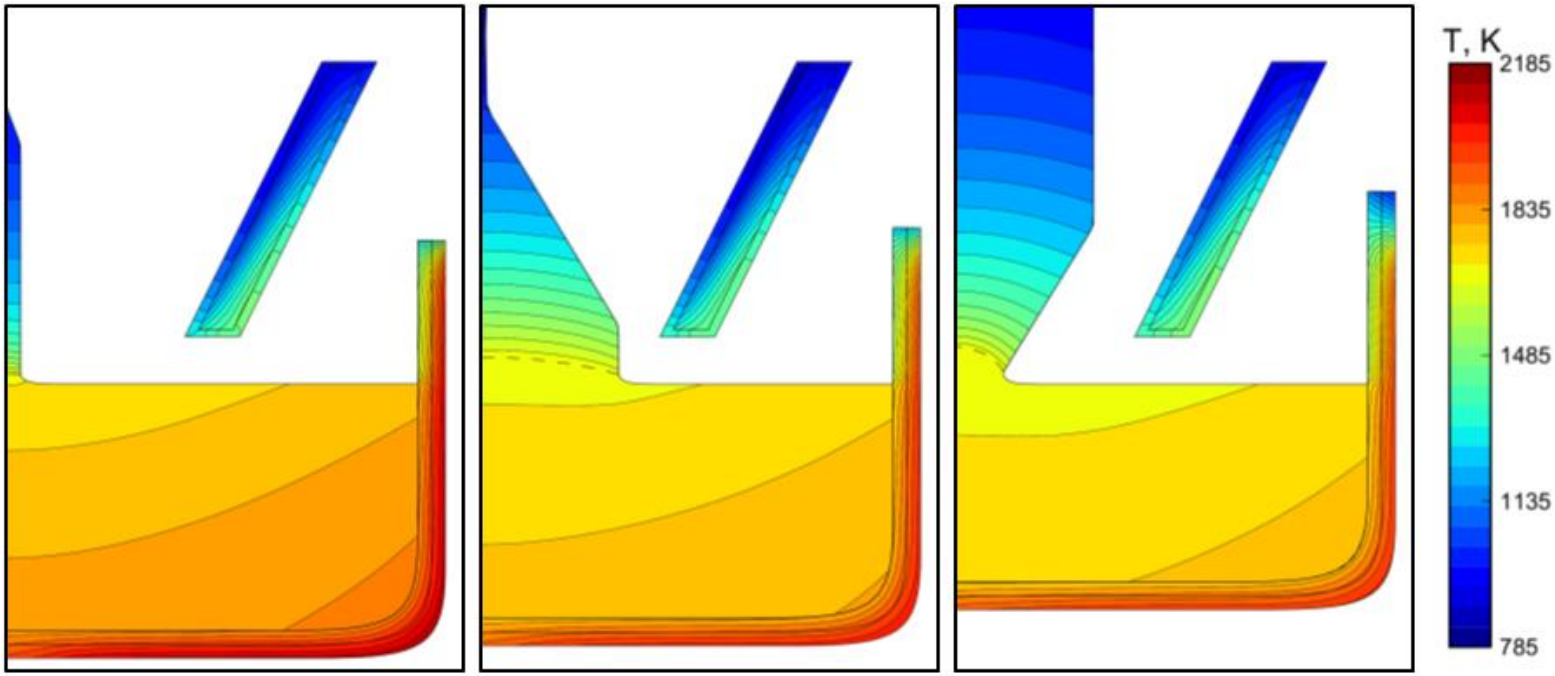


- For the whole growth process the pull rate of 1 mm/min was used as a setpoint
- PID controller for pull rate used crystal radius deviation as an input
- PID controller for heater power used pull rate deviation as an input

Calculation example

Key of success - optimal heater power curve

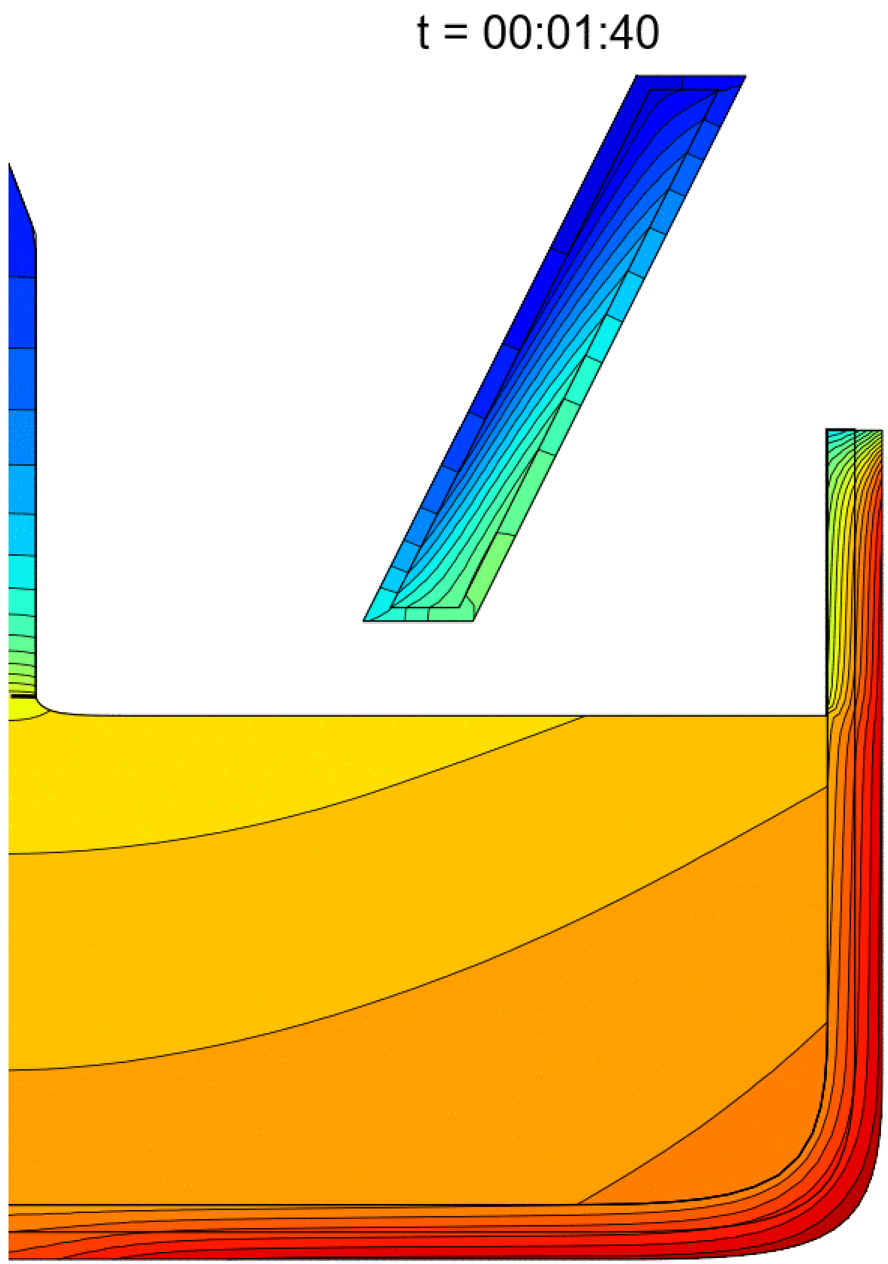
- For a successful simulation, it was necessary to obtain an optimal heater power curve. This process is described in the next slides



Calculation example

Full growth process

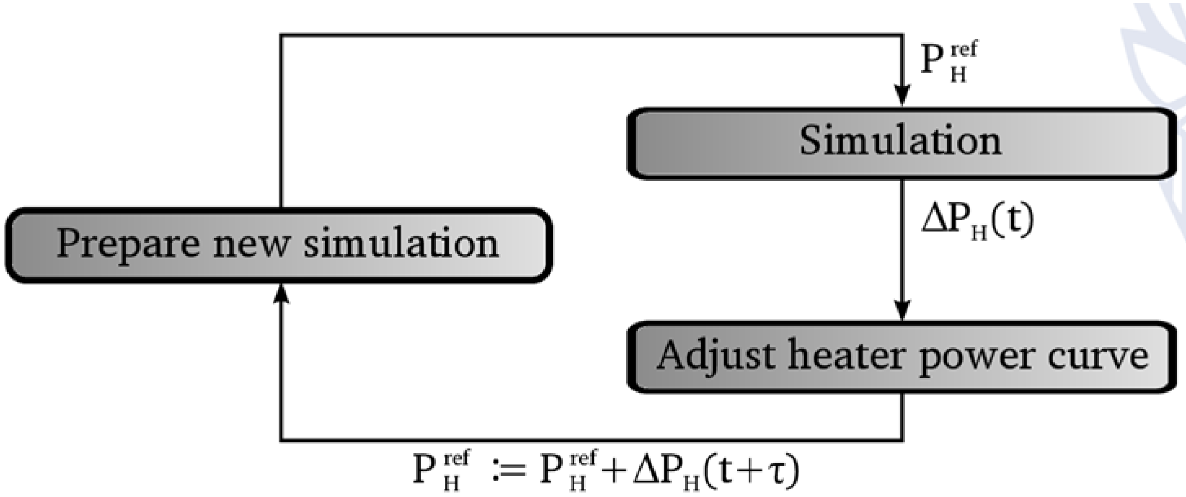
- Seeding and Dash neck at 0:00
- Start cone at 2:10
- Shouldering at 5:30
- End cone at 9:30



Calculation example

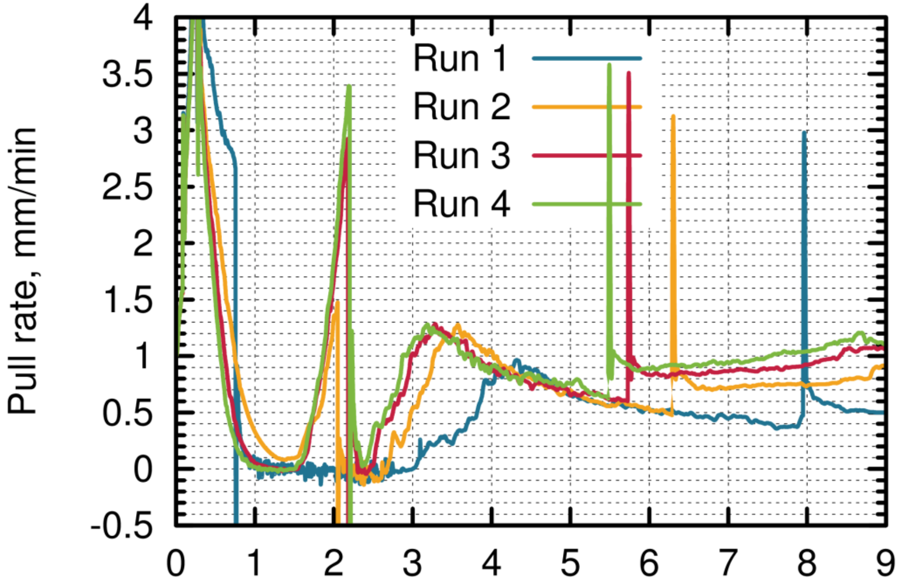
Obtaining optimal heater power curve

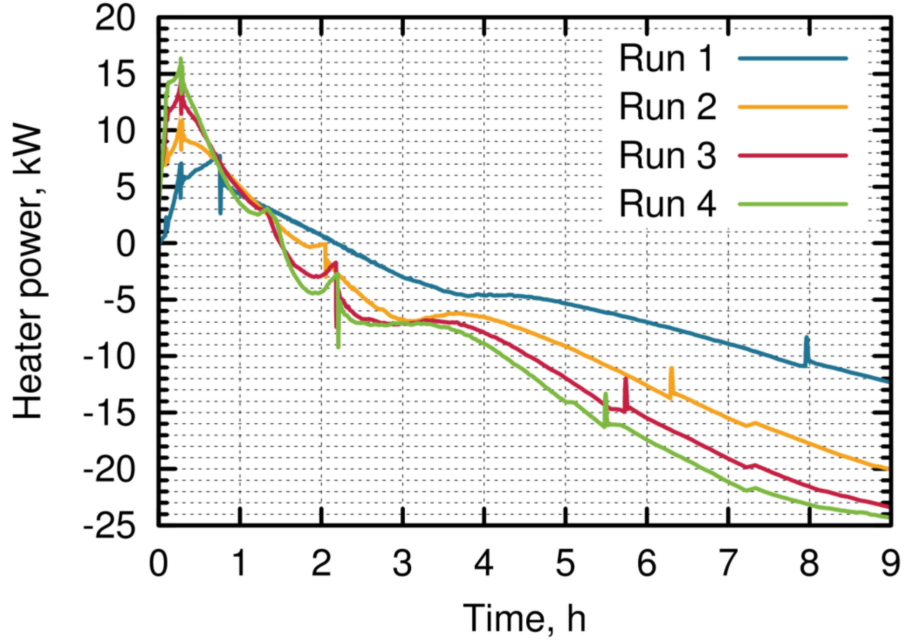
- Repeated calculations were carried out, using a reference power curve obtained from the previous calculation
- To accommodate the thermal inertia of the melt, this power curve was shifted towards smaller time values by τ =40 min

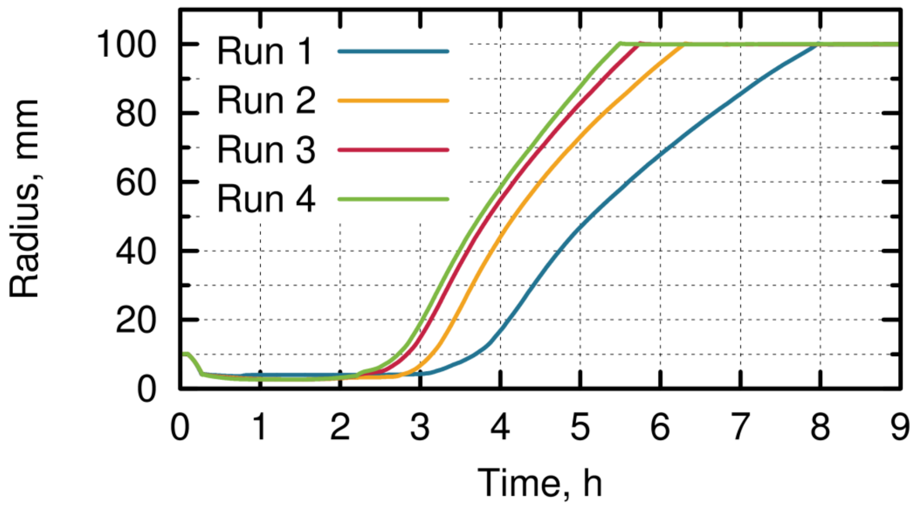


Calculation example

Start cone growth – functions of time





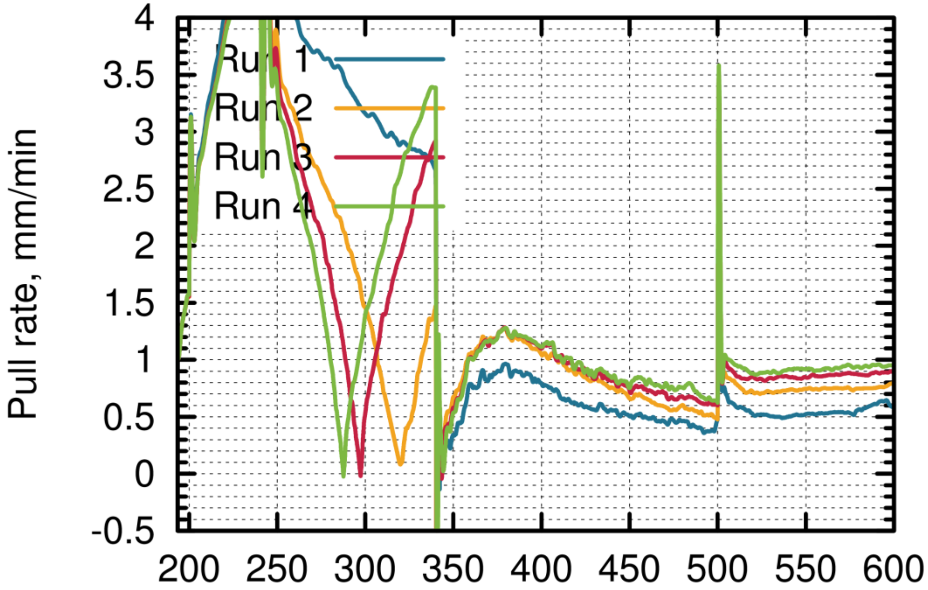


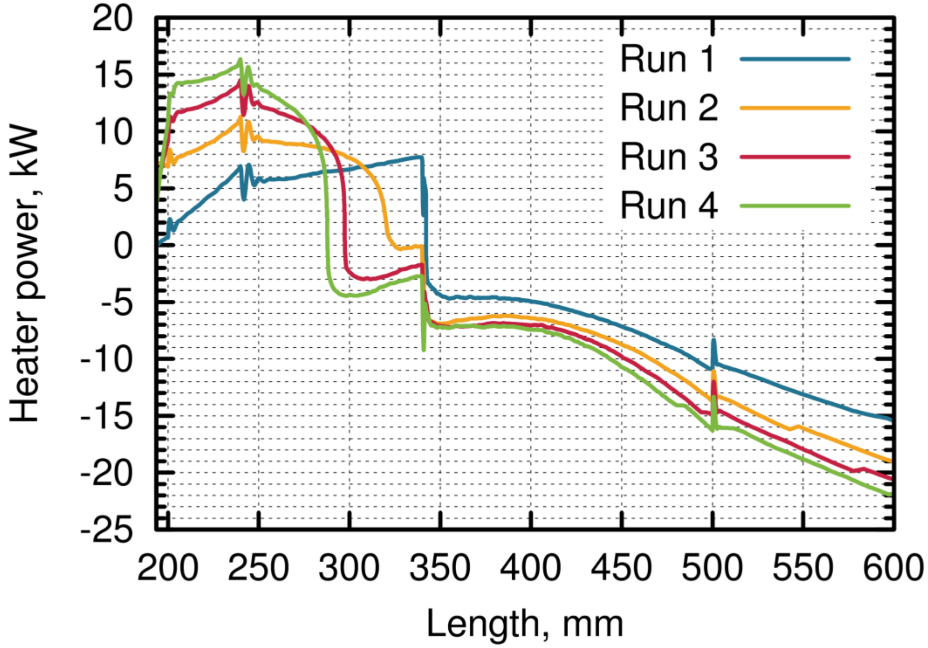
Run 0: P_ref(t)==0 kW
P(t)=P_ref(t) + ΔP_PID(t)

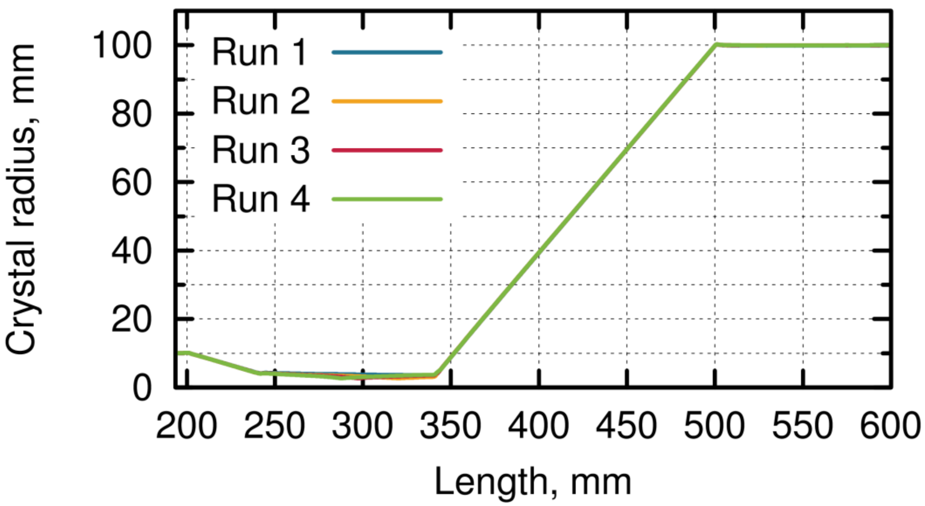
- Calculation parameters show a tendency to converge, i.e. the difference between parameter changes decreases for each next run

Calculation example

Start cone growth – functions of crystal length



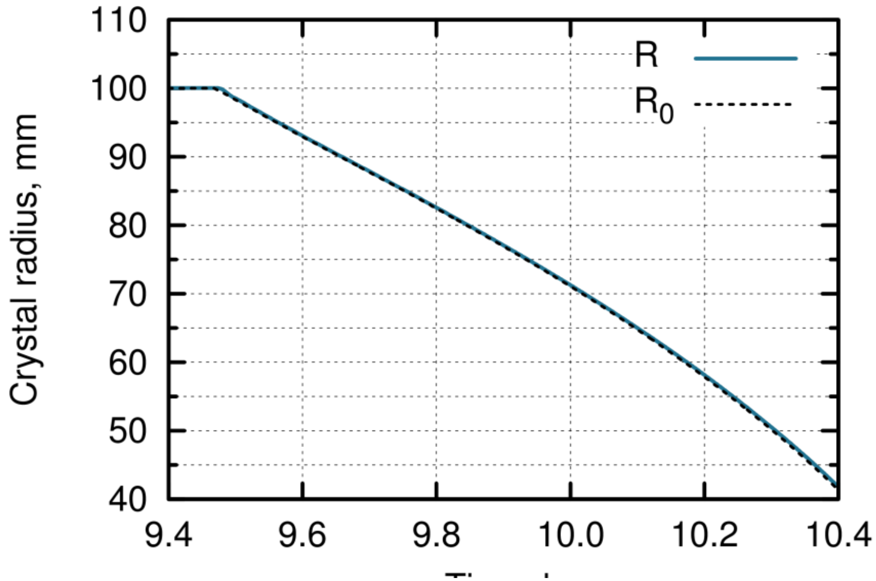




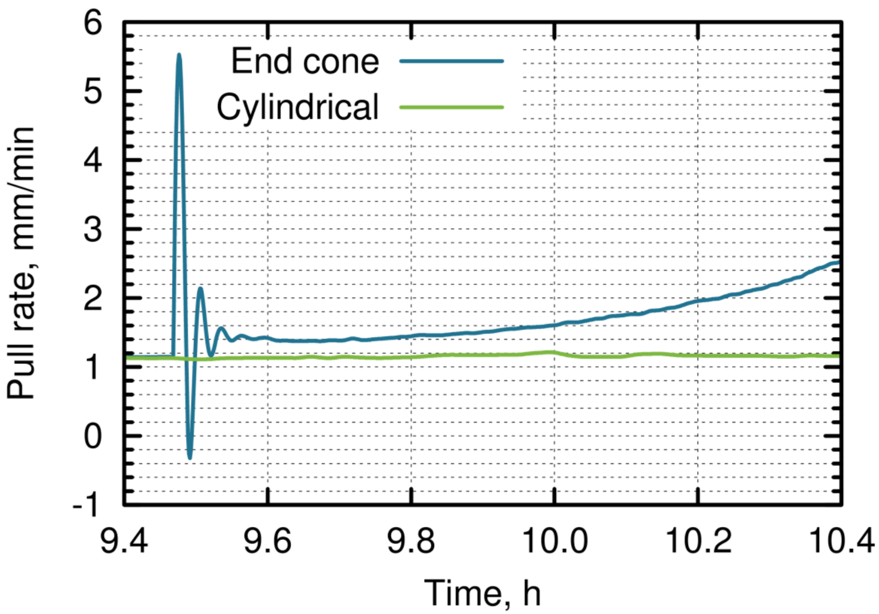
- Shape has higher priority than growth rate
- Pull rate is closer to 1 mm/min in optimized runs

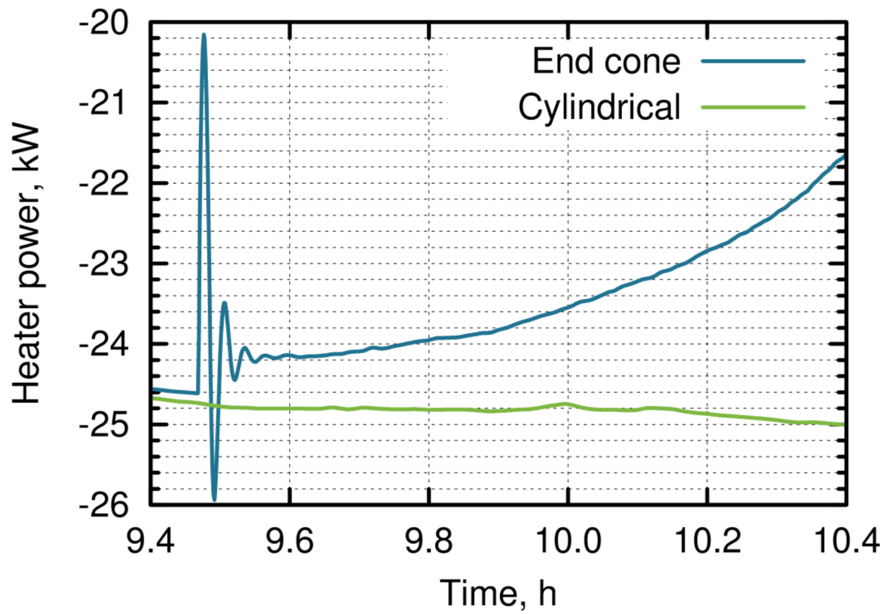
Calculation example

End cone growth



- After successfully optimizing the growth for the start cone and obtaining a 250 mm cylindrical ingot, the end cone was grown (started at 9.45 h)





Conclusions

- Full CZ growth modelling has been performed using the developed mathematical model and software
- An optimal power curve for the start cone growth was obtained by performing repeated simulation runs
- With the optimal power curve, cone part was grown 2.5 h faster than without it
- However, further investigation is necessary to determine the optimal controller parameters for the different process stages.

Process control

- PID controller: $\Delta u(t) = K_p \left(e(t) + T_d \frac{de}{dt}(t) + \frac{1}{T_i} \int_0^t e(\tau)\, d\tau \right)$, $e(t) = f_0(t) - f(t)$, $u(t) = u^{\mathrm{ref}}(t) + \Delta u(t)$.

Crystal pull rate	Heater power
$K_p = -3\,\mathrm{min}^{-1}$,	$K_p = -1\,\mathrm{kW} \cdot \mathrm{min/mm}$,
$T_i = \infty$, $T_d = 130\,\mathrm{s}$	$T_i = 1000\,\mathrm{s}$, $T_d = 0$