

Pharmaceutical  
Multiphase Reactors  
CHE.782

Design of Multiphase  
Flow Processes  
669.266

## Hands on the „ParScale“ Library

- A - Modify an existing case
- B - Extend an existing case

Ass.Prof. Dr. Stefan Radl,  
M. Sc. Thomas Forgber  
Email: [radl@tugraz.at](mailto:radl@tugraz.at)  
Institute of Process and  
Particle Engineering  
Inffeldgasse 13/III  
TU Graz

A part of this teaching material has been  
prepared for NanoSim (<http://sintef.no/NanoSim/>)



NanoSim - A Multi-scale Simulation-Based Design Platform

### Where to find:

- Verification case:  
„*examples/verificationCases/heatConductionTransientBC*“

### What to do:

- Run the existing verification case
- **Modify** it by:
  - (1) Track a second particle with  $T_0 = 500$  K and  $T_{\text{eviro}} = 800$ K
  - (2) Double the radius of the second particle
  - (3) Use 20 grid points per particle
  - (4) Double the liquid and gas phase fraction
  - (5) Make the simulation run twice as long without producing more data
  - (6) Visualize both particle temperatures in one plot

(1) Track a second particle with  $T_0 = 500$  K and  $T_{\text{eviro}} = 800$  K

- Edit the input file (number\_particles)
- Add a second line to all files the „0/“ folder
- Set the temperature of the second particle

(2) Double the radius

- Edit the „0/radius.json“ file

(3) Use 20 grid points per particle

- Edit the input file (nGridPoints)
- Edit all files the the „0/“ folder according to your new number of grid points

(4) Double the liquid and gas phase fraction

- Edit „gasPhaseFraction.json“/“liquidPhaseFraction.json“ in your „0/“ folder

(5) Make the simulation run twice as long without producing more data

- Edit the input file (control section)
- Adjust „control run“ and „outputTimeStep“

(6) Visualize both particle temperatures in one plot

- Understand and edit all post processing routines in the „octave/“ folder

### Where to find:

- Verification case:  
*„examples/verificationCases/heatConductionTransientBC“*
- Extend by adding a reaction similar to  
*„examples/verificationCases/nonCatalyticHeterogeneousReaction “*

### What to do:

- Run the existing verification case
- **Extend** it by:
  - (1) Add a new species equation
  - (2) Add a new reaction that consumes the species, and which is temperature depended (but does not release heat)
  - (3) Ramp up the temperature by using the „JSON“ coupling option
  - (4) Visualize the temperature and concentration field in a single plot

### (1) Add a new species equation

- Edit the input file (model section, all relevant models parameters)
- Add a files the „0/“ folder which is named after you species and define the initial conditions (concentration)

### (2) Add a new reaction that consumes the species, and which is temperature depended (but does not release heat)

- Edit the input file (add single reaction chemistry model)
- Add single reaction file in the „settings/“ folder according to the requirements (“isIsoThermal”, “Arrhenius\_A”, “names”)

### (3) Ramp up the temperature by using the „JSON“ coupling option

- Edit the input file (add coupling model json)
- Add coupling model json file in “settings/”- folder (see existing settings folder for template)

(4) Visualize the temperature and concentration field in a single plot

- Understand and edit all post processing routines in the „octave/“ folder

# Impressum & Disclaimer

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