



Modular, scalable and high-performance
DE-polymerization by MicrowavE TechnolOgy

State-Space Thermal Modeling of a Depolymerisation Reactor

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- Main issue:

DEMETO employs a depolymerisation reactor based on microwaves. The reactor structure, the temperature and the electric field make difficult to measure the mixture temperature because sensors would operate under harsh conditions.

- Main goal:

Provide a physical model of the reactor able to estimate the temperature of the mixture in order to implement a control chain to supervise the process.

- DEMETO solution:

The solution is based on a state-space model that acts as a kind of simplified FEM. The aim is to model the reactor and observe its internal state to observe and forecast the behaviour with a defined setup or even to directly control the temperature.

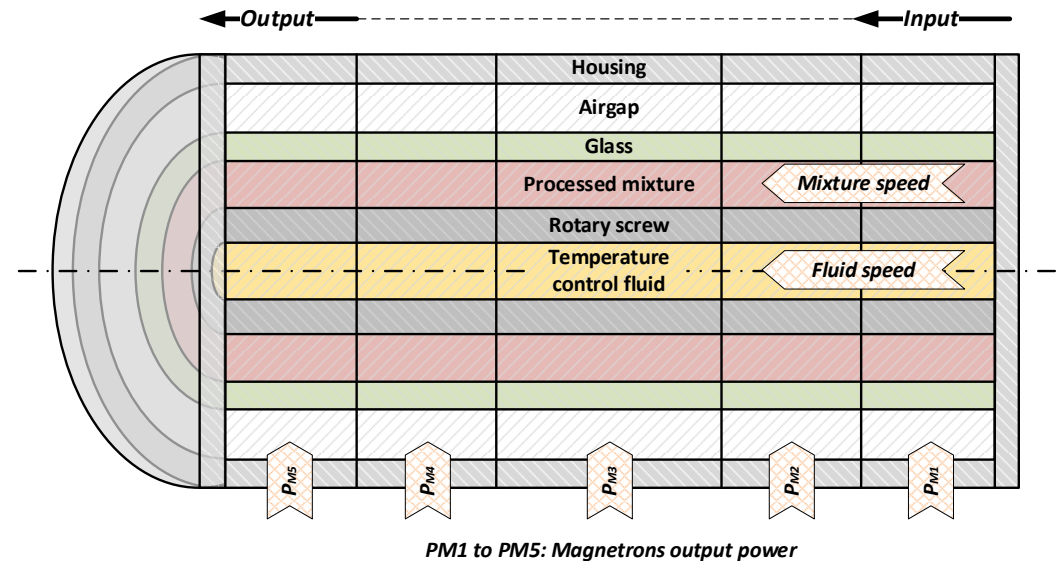
Structure of the reactor and input parameters

Particularities of the reactor geometry:

- The reactor has an axisymmetric structure with 5 reaction chambers.
- All axial layer are solid and static materials except for the 'Processed mixture' layer and the 'Temperature control fluid' layer. These materials move axially during the process.

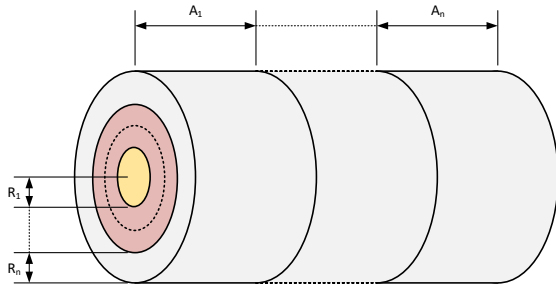
Inputs parameters

- P_{M1} to P_{M5} : power delivered by the magnetrons.
- Mixture speed.
- Fluid speed
- Boundaries conditions (ambient air)

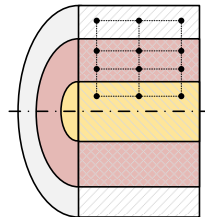


Thermal model: From structure to elements

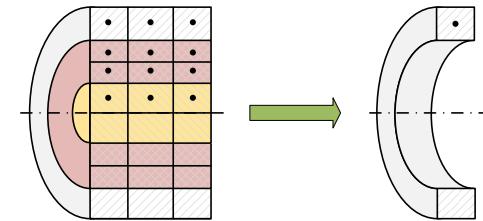
1. The reactor is axisymmetric and its structure has a configurable number of axial and radial layers.



2. Each layer is meshed radially and axially with an adaptive mesh which is configurable section by section.

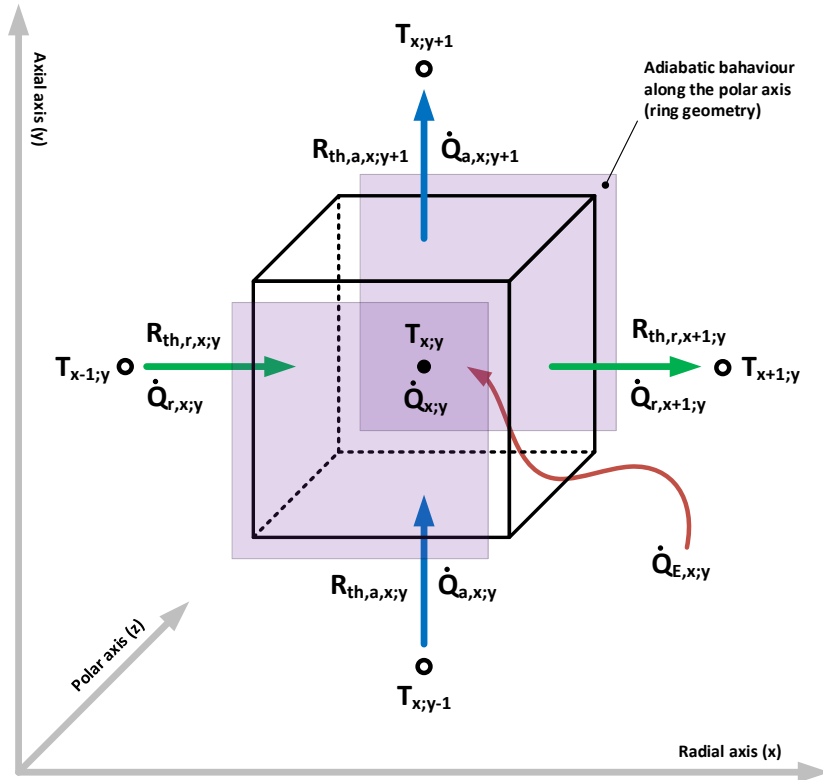


3. Each mesh point represents a ring shape element with homogenous properties and temperature.



4. The polar integration of the elements properties is done considering their axial and radial coordinates and the resulting contact surfaces.

Thermal model: Mathematical description of each element



Radial heat exchange (conduction):

$$\dot{Q}_{r,x;y} = \frac{T_{x-1;y} - T_{x;y}}{R_{th,r,x;y}}$$

$$\dot{Q}_{r,x+1;y} = \frac{T_{x;y} - T_{x+1;y}}{R_{th,r,x+1;y}}$$

Axial heat exchange (cond. & mass flow):

$$\dot{Q}_{a,x;y} = \frac{T_{x;y-1} - T_{x;y}}{R_{th,a,x;y}} + v_a \cdot S_{a,y} \cdot c_{x;y} \cdot \rho_{x;y} \cdot T_{x;y-1}$$

$$\dot{Q}_{a,x;y+1} = \frac{T_{x;y} - T_{x;y+1}}{R_{th,a,x;y+1}} + v_a \cdot S_{a,y} \cdot c_{x;y} \cdot \rho_{x;y} \cdot T_{x;y}$$

The main equation that governs the heat exchanges is:

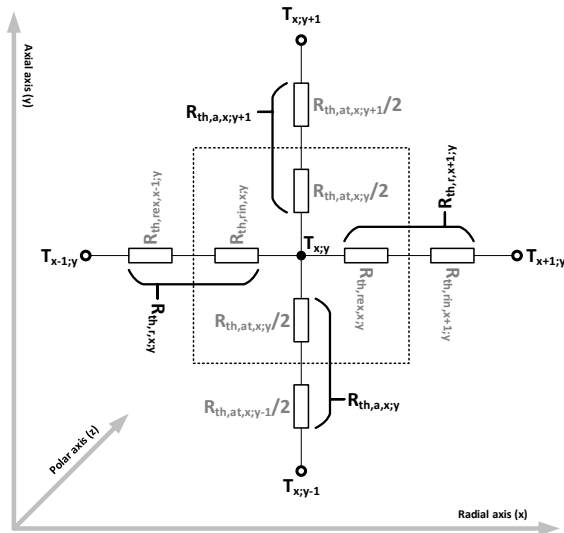
$$\dot{Q}_{x;y} = \dot{Q}_{E,x;y} + \dot{Q}_{r,x;y} + \dot{Q}_{a,x;y} - \dot{Q}_{r,x+1;y} - \dot{Q}_{a,x;y+1}$$

Microwaves and reaction heating:

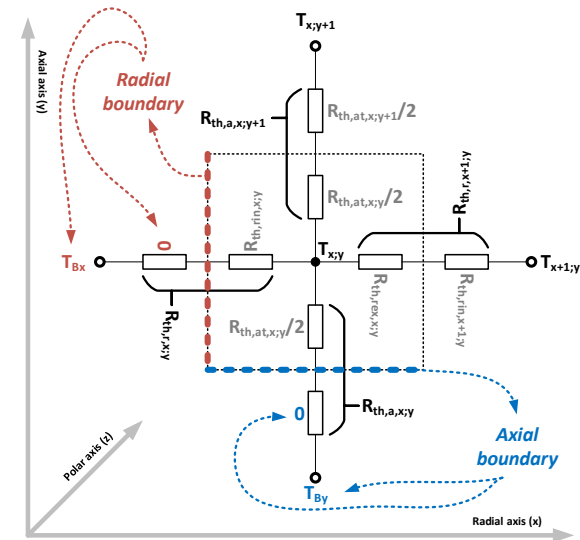
$$\dot{Q}_{E,x;y} = \frac{V_{x,y}}{V_i} \cdot (\dot{Q}_{MW,i} + \dot{Q}_{R,i}) = \frac{V_{x,y}}{V_i} \cdot \dot{Q}_{E,i}$$

Thermal model: Domain boundary conditions

Element *without* boundary conditions



Element *with* boundary conditions



When boundary (radial or axial) touches an element, two conditions change:

- Thermal resistance outside the boundary is considered being null
- A boundary temperature is fixed

Thermal model: State-space representation and simulation

The mathematical model gives the following equation common for each element:

$$\dot{T}_{x;y} = \frac{1}{m_{x;y} \cdot c_{x;y}} \cdot \left(\frac{V_{x,y}}{V_i} \cdot \dot{Q}_{E,i} + \frac{T_{x-1;y}}{R_{th,r,x;y}} + \frac{T_{x+1;y}}{R_{th,r,x+1;y}} + \frac{T_{x;y+1}}{R_{th,a,x;y+1}} + T_{x;y-1} \cdot \left(\frac{1}{R_{th,a,x;y}} + v_a \cdot S_{a,y} \cdot c_{x;y} \cdot \rho_{x;y} \right) \right)$$

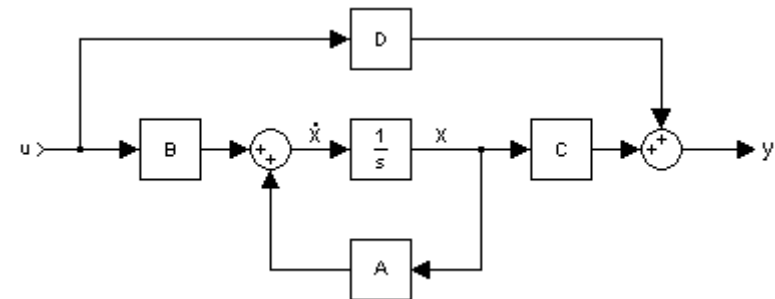
Main statements:

- All fluids are considered as solids, to consider convection, thermal resistor must be adapted
- Mass flow is considered as constant in order to keep the system linear

With the equation of the system, is possible to build the state-space representation of the system in the following form:

$$\begin{cases} \dot{x} = Ax + Bu \\ y = Cx + Du \end{cases}$$

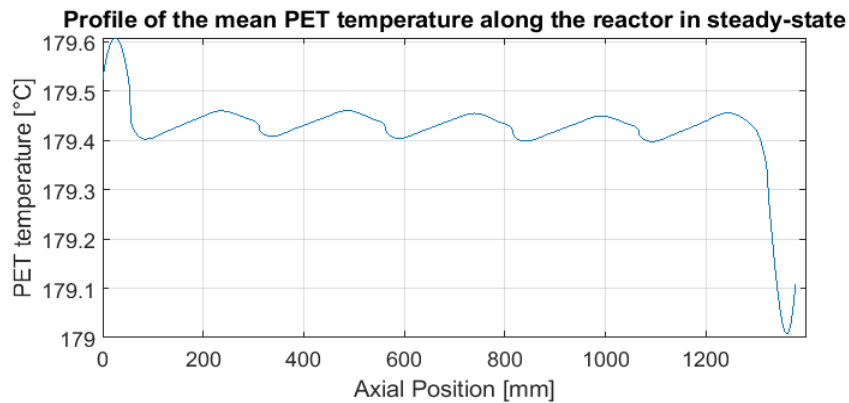
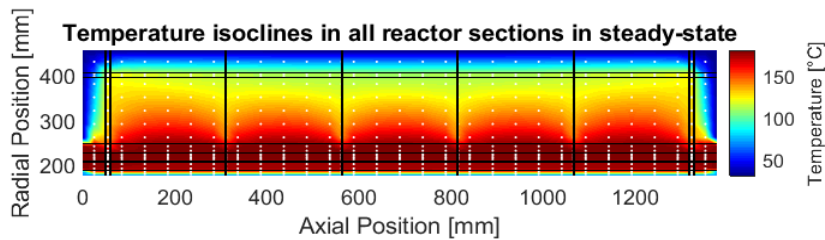
Once that the matrix are built, the system is simulated using Simulink:



Thermal model: Simulation examples

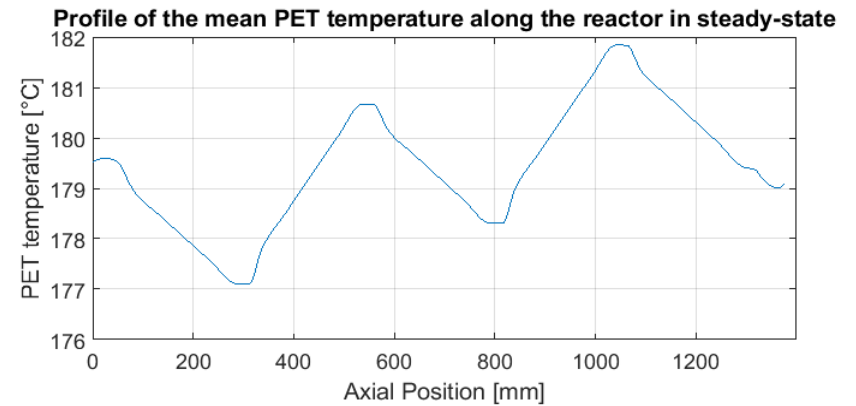
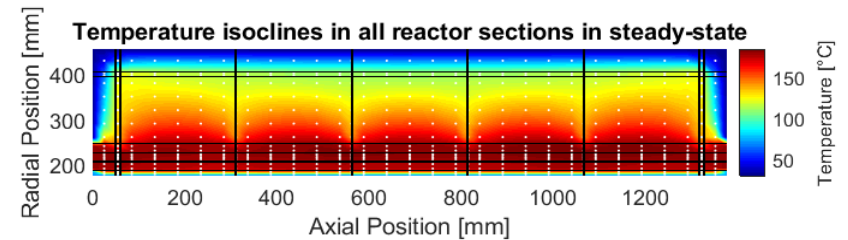
Example N°1:

Magnetrons power: all at 400W



Example N°2:

Magnetrons power: P_{M2} and P_{M4} at 1000W



- Results validation:

The model has been validated using a FEM standard tool (Ansys FLUENT), which considers also radiation and convection phenomena. An error of ± 3 [°C] has been observed and the dynamic of the model corresponds.

- Temperature control:

This model can be employed to forecast the temperature or control it in the reaction chamber after a model reduction procedure.

- Extend to others systems:

This model can be easily be adapted to others geometries changing the geometry and mesh definition.

