Thermochemical analysis of a packed-bed reactor using finite elements with FlexPDE and COMSOL Multiphysics

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**Supplementary material**

**APPENDIX A**

**CALCULATION OF THE SPEED OF EACH COMPONENT AND THE REACTION HEAT**

Reaction Stoichiometry:

|  |  |
| --- | --- |
| $$CO + (2+1/n)H\_{2}\rightarrow (1/n)C\_{n}H\_{2n+2}+H\_{2}O H\_{r}=-165kJ$$ | (A1) |
| $$CO+3H\_{2}\rightarrow CH\_{4}+H\_{2}O ΔH\_{r}=-215kJ$$ | (A2) |

Reaction Rate of Monoxide and Methane

|  |  |
| --- | --- |
| $$-r\_{co}=\frac{(1-β\_{co}t)A\_{co}^{`'}e^{Eco/RT\_{o}(\frac{1-θ}{θ})}y\_{co}y\_{H2}}{(1+K\_{co}y\_{co})^{2}}$$ | (A3) |
| $$r\_{CH\_{4}}=\frac{(1-β\_{CH4}t)A\_{CH\_{4}}^{'}e^{E\_{CH\_{4}}/RT\_{o}(\frac{1-θ}{θ})}y\_{CO}^{^{1}/\_{2}}y\_{H\_{2}}}{(1-K\_{co}y\_{co})^{2}}$$ | (A4) |

Schulz-Flory-Anderson distribution

|  |  |
| --- | --- |
| $r\_{n}=r\_{3}α^{n-3}$ , n≥3 ; C2/C3 = $γ$ | (A5) |

According to the stoichiometry of the Reaction:

|  |  |
| --- | --- |
| $$r\_{H\_{2}0}=-r\_{CO}$$ | (A6) |

Carbon Balance:

|  |  |
| --- | --- |
| $$r\_{co}+r\_{CH\_{4}}+2r\_{2}+\sum\_{n=3}^{1}nr\_{n}=0$$ | (A7) |

Hidrogen Balance:

|  |  |
| --- | --- |
| $$r\_{H\_{2}}+r\_{H\_{2}o}+2r\_{CH\_{4}}+3r\_{2}+\sum\_{n=3}^{1}(n+1)r\_{n}=0$$ | (A8) |

Replacing A5 in A7 and A8

|  |  |
| --- | --- |
| $$r\_{co}+r\_{CH\_{4}}+2γr\_{3}+r\_{3}\sum\_{n=3}^{1}nα^{n-3}=0$$ | (A9) |
| $$r\_{H2}-r\_{co}+2r\_{CH\_{4}}+3γr\_{3}-r\_{3}\sum\_{n=3}^{1}(n+1)α^{n-3}=0$$ | (A10) |

The Summation factor can be replaced by

|  |  |
| --- | --- |
| $$S\_{1}=\sum\_{n=3}^{1}nα^{-3}=\frac{3-2α}{(1-α)^{2}}$$ | (A11) |
| $$S\_{2}=\sum\_{n=3}^{1}(n+1)α^{n-3}=\frac{4-3α}{(1-α)^{2}}$$ | (A12) |

r3 y $r\_{H\_{2}}$from A9 and A10

|  |  |
| --- | --- |
| $$r\_{3}=-\frac{r\_{co}+r\_{CH\_{4}}}{2γ+S\_{1}}$$ | (A13) |
| $$r\_{H\_{2}}=-\left[-r\_{co}+2r\_{CH\_{4}}+r\_{3}(3γ+S\_{2})\right]$$ | (A14) |
| $$(-ΔH)r\_{v}=215000r\_{CH\_{4}}-165000(r\_{CO}+r\_{CH})$$ | (A15) |

rn can be calculated fromde AI 5, r2=γr3 and $r\_{H\_{2}O}=-r\_{CO}$ (A16)

**APPENDIX B**

**CALCULATION OF THE TOTAL HEAT TRANSFER COEFFICIENT UC**

If the wall thickness is considerable and the heat transfer through the wall decreases, it is advisable to use the through-wall conduction model. However, it is possible to calculate a global heat transfer factor Uc which considers the heat transfer through the wall and the convention with the cooling fluid and translate it to the homogeneous dynamic model instead of the value of αw.

The calculation is as follows:

Heat Balance in Tube Thickness:

|  |  |
| --- | --- |
| $$λ\_{w}\frac{1}{r}\frac{∂}{∂r}(r\frac{∂T}{∂r})=0$$ | (B1) |

Border Conditions:

|  |  |
| --- | --- |
| $$λ\_{cr}\frac{∂T}{∂r}\left|r=R=\left.λ\_{w}\frac{∂T}{∂r}\right|\right.\_{r=R}$$ | (B2) |
| $$-λ\_{w}\frac{∂T}{∂r}\left|r=RO\right.=α\_{w}(T\_{RO}-T\_{C})$$ | (B3) |

From equation A1

|  |  |
| --- | --- |
| $$T=C\_{1}lnr+C\_{2}$$ | (B4) |
| $$\frac{∂T}{∂r}=\frac{C\_{1}}{r}$$ | (B5) |

From equation B4 with border conditions: $T\_{R\_{0}}$when r=Ro and TR when r=R

|  |  |
| --- | --- |
| $$T\_{R\_{0}}=C\_{1}ln(R\_{0}/R)+T\_{R}$$ | (B6) |

C1 es calculated replacing $T\_{R\_{0}}$ from B6 in B3 y $\frac{∂T}{∂r}$ from B5 in B3 we obtain C1

|  |  |
| --- | --- |
| $$-C\_{1}=\frac{α\_{w}}{λ\_{w}}\left[\frac{1}{R\_{0}}+\frac{α\_{w}}{λ\_{w}}ln(\frac{R\_{0}}{R})\right]^{-1}(T\_{R}-T\_{c})$$ | (B7) |

Replacing B2 in B5 using expression B7

|  |  |
| --- | --- |
| $$-λ\_{cr}\frac{∂T}{∂r}\left|r=R\right.=\frac{α\_{w}}{R}\left[\frac{1}{R\_{0}}+\frac{αw}{λ\_{w}}ln(\frac{R\_{O}}{R})\right]^{-1}(T\_{R}-T\_{c})$$ | (B8) |
| $$-λ\_{cr}\frac{∂T}{∂r}\left|r=R\right.=U\_{c}(T\_{R}-T\_{c})$$ | (B9) |

Being:

|  |  |
| --- | --- |
| $$U\_{c}=\frac{α\_{w}}{R}\left[\frac{1}{R\_{0}}+\frac{αw}{λ\_{w}}ln(\frac{R\_{O}}{R})\right]^{-1}$$ | (B10) |

**APPENDIX C**

**OPTIMAL MESH NUMBER DETERMINATION**

Table C1. Element size and Mean-Absolute-Error (MAE) of the mesh types considered.

|  |  |  |
| --- | --- | --- |
| **Mesh Type** | **Element size (m)** | **MAE** |
| Extremely fine | 0.0300 | 1.60 |
| Finer | 0.0825 | 2.24 |
| Normal | 0.1500 | 4.32 |
| Coarser | 0.2850 | 235.28 |

**APPENDIX D**

**CONCENTRATION, TEMPERATURE AND REACTION RATE PROFILES IN 3D**

# Chart  Description automatically generated

Figure D1. CO concentration (mol/m3)



Figure D2. CH4 concentration (mol/m3)



Figure D3. Temperature (K)



Figure D4. CO Reaction Rate (mol/kgcat s)