

DWSIM Simulation Project

Topic of Simulation:

- Sulphuric Acid Proces

Group Members & Contribution:

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Description:

Started with liquid Sulfur and Oxygen, combustion using conversion reactor, conversion to SO₃ using 1 PFR which simulated reaction kinetics and 1 downstream conversion reactor for residual conversion, followed by downstream separations and absorption reaction to form pure H₂SO₄ (liquid) as product.

Reaction Kinetics:

Under 'Reactions Manager', the reaction used for SO₂ → SO₃ is the one labelled 'New hetcat', a heterogeneous catalytic type reaction.

Rate law is of the form:

Numerator: $(775 \cdot \exp(-22000/(1.98 \cdot T))) \cdot R_1 \cdot R_2 \cdot (1 - (P_1/R_2/(R_1^{0.5})/(10^{(500/T-4.743)})))^2$

Denominator: $(R_1 + 0.8 \cdot P_1)$

Where R₁ = partial pressure of O₂, R₂ = partial pressure of SO₂, P₁ = partial pressure of SO₃

The kinetics was as proposed by G. K. Boreskov.

Reference:

Kinetics and effectiveness factor for SO₂ oxidation on an industrial vanadium catalyst, H. Livbjerg , J. Villadsen, Chem. Engg. Sci., Volume 27, **21-38**, (1972)

Relevant areas in the paper: Table 1 entry 3, Eqns 6 ,7,8, Tables 5 and 8 for calculation of rate constant expression