

AROM-SIM™

Reactor Models for Petrochemical Processes

a KBC SIM Model

AROM-SIM is the KBC family of reactor models that simulate xylene isomerisation and aromatics transalkylation. These reactors, along with other standard Petro-SIM™ unit operations, can provide you with a detailed model of aromatics processing facilities.

The isomerisation of C₈ aromatics into paraxylene is performed using the AROM-SIM Xylene Isomerisation reactor model. It can model technologies such as Isomar™, XyMax™, and Oparis™ (licensed by UOP, Exxon Mobil Corporation, and Axens respectively) among other licensor technologies. The model includes both mechanisms for transalkylation of ethylbenzene (EB) to xylenes and dealkylation of EB to benzene.

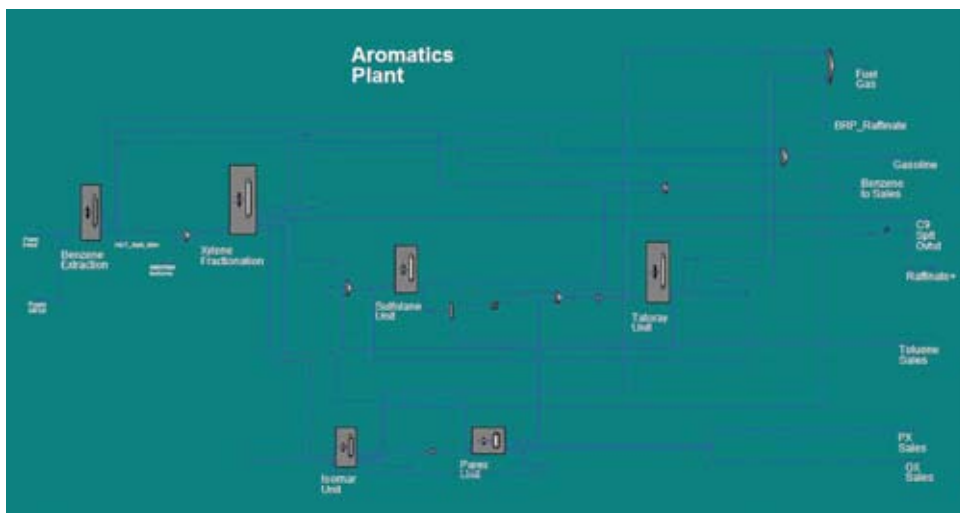
Transalkylation processes are modelled with the Aromatics Transalkylation reactor model. This model is capable of emulating all commercial transalkylation processes such as UOP Tatoray™, THDA, and PX-Plus™ as well as Exxon Mobil Corporation/Axens TransPlus™, PxMax™ among other licensor technologies. The model includes kinetic reactions for dealkylation, toluene disproportionation and C₉/C₁₀ aromatics transalkylation, plus the many additional reactions that take place.

For specified feeds, operating conditions, and constraints, the program determines resulting product flows and compositions as well as overall unit operating economics.

FEATURES

AROM-SIM contains the following key features:

- Kinetic model consisting of primary and side reaction equations for isomerisation and transalkylation
- Linear or weighted distribution of energy use along the reactor



Aromatics Flowsheet

- Auto-tuning or manual tuning capability
- Detailed compositional model output with stream properties
- Case studies and optimisation capabilities to determine maximum performance
- Easy to use LP Data Utility to create LP shift vectors and submodels
- Integration with other refinery units using Petro-SIM, to model interaction between these units, reformers, and other key operations

Petro-SIM FLOWSHEET

AROM-SIM is available within Petro-SIM and Petro-SIM Express, the KBC process flowsheet simulator. You can model each reactor as an individual unit, model them in the same flowsheet or model with upstream and downstream units to determine key interactions over a section or the entire facility.

(Continued)

BENEFITS

AROM-SIM is a decision support tool to help answer the following questions:

- **Selection of Operating Targets** – How do I maximise the amount of paraxylene? What is the effect of ethylbenzene conversion on xylene isomerisation? How can I best control the amount and quality of recycle?
- **Evaluation of New Feedstocks or Upstream Operations** – What are the effects of a new feed on product qualities and yields? How does a change in feed naphthenes affect my process? What are the best feedstocks to the transalkylation unit?
- **LP Submodel Generation** – What vectors are needed in the linear program (LP) to model the incremental yields for different feeds and operating conditions?
- **Debottlenecking** – What are the economic effects of increasing the Hydrogen to hydrocarbon ratio? What are the effects of changing reactor pressures or conversion levels?
- **Training** – How do I get new engineers and operators up to speed?
- **Design** – What is the best configuration for a new facility?

Xylene Isomerisation Reactor

Performance	Isom Feed	Isom Reactor Effluent	Conversion
Overall	10.5451	8.3216	21.1
Composition	0.0000	0.0000	
Plots	123.5586	39.8033	67.8
Conversion	49.3723	525.5754	-964.5
	1720.3397	1255.0337	27.0
	659.2285	553.5411	16.0
	9.3918	8.1638	13.1
	0.0000	0.0000	
	0.0586	0.0586	-0.0
	0.6274	49.4021	-7773.8
	0.0000	0.0000	
	0.5768	0.5768	0.0
	0.0000	0.0000	

Design Rating Calibration Factors Worksheet Performance

Aromatics Isomerisation Reactor

Aromatics Transalkylation Reactor

Rating	Reactions	ID	Active
Setting	2 Toluene ↔ m-Xylene + Benzene	112	<input checked="" type="checkbox"/>
Components	E-Benzene + H2 ↔ Benzene + Ethane	113	<input checked="" type="checkbox"/>
Reactions	2 m-Xylene ↔ 1,2,3-Mbenzene + Toluene	114	<input checked="" type="checkbox"/>
Profile	E-Benzene + m-Xylene ↔ 1,3,5-EBenzene + Toluene	115	<input checked="" type="checkbox"/>
Solver	E-Benzene + m-Xylene ↔ m-Pbenzene + Toluene	116	<input checked="" type="checkbox"/>
	E-Benzene + 1,3,5-EBenzene ↔ m,DiE-Benzene + Toluene	119	<input checked="" type="checkbox"/>
	m-Pbenzene + m-Xylene ↔ m-Tbenzene + Toluene	120	<input checked="" type="checkbox"/>
	1,4-EBenzene + H2 ↔ EBenzene + Ethane	121	<input checked="" type="checkbox"/>
	1,4-DiPropylBZ + H2 ↔ Toluene + Propane	122	<input checked="" type="checkbox"/>
	1-c3MCCS + H2 ↔ Nonyclohexane + Methane	123	<input checked="" type="checkbox"/>

Design Rating Calibration Factors Worksheet Performance

Aromatics Transalkylation Reactor

PREDICTIVE TECHNOLOGY FOR PROFIT IMPROVEMENT

- Petro-SIM™ for Process Simulation
- Petro-SIM Express™ for Process Simulation
- KBC SIM Suite:
 - FCC-SIM™ for Fluid Catalytic Cracking
 - REF-SIM™ for Catalytic Reforming
 - HCR-SIM™ for Hydrocracking
 - N HTR-SIM™, D HTR-SIM™ and VGO HTR-SIM™ for Hydrotreating
 - DC-SIM™ for Delayed Coking
 - VIS-SIM™ for Visbreaking and Thermal Cracking
 - ALK-SIM™ for Alkylation
 - RHDS-SIM™ for Residue Hydrotreating
 - AROM-SIM™ for Aromatics
 - ISOM-SIM™ for Isomerisation
 - Olefin-SIM™ for Pyrolysis



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