SIMULATION OF PRESSURE SWING ADSORBER REACTOR FOR ISOMERIZATION OF N-PARAFFINS

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MASTER OF SCIENCE
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DEDICATION

To my parents

Abstract of thesis presented to the Senate of Universiti Putra Malaysia in fulfilment of the requirements for the degree of Master of Science

SIMULATION OF PRESSURE SWING ADSORBER REACTOR FOR ISOMERIZATION OF N-PARAFFINS

By

LAI YIN LING

October 2004

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In this thesis, a non-isothermal pressure swing adsorber-reactor (PSAR) model for the isomerization of n-paraffins is developed. PSAR is a new concept that combines the isomerization of normal paraffins to iso-paraffins and separation of the iso-paraffins from mixtures of n/iso-paraffins by using pressure swing adsorption (PSA). The isomerization of normal-pentane (n-C_5) to iso-pentane (i-C_5) is used to illustrate the concept of PSAR. The PSAR column is packed with a layer of catalyst (Y-zeolite) and followed by a layer of adsorbent (zeolite 5A). The mathematical model is solved numerically using the method of lines where the partial differential equations (PDEs) are partially discretized and reduced to ordinary differential equations (ODEs). Orthogonal collocation (OC) method is used as the discretization method. The computer programme is written in FORTRAN 99.

The numerical implementation of the developed PSAR is verified by adjusting the ratio of the length of the reactor section to the total length of the PSAR column, ω. When ω approaches 0, the PSAR model is reduced to PSA separation model. When ω approaches 1, the model is reduced back to steady state reactor model. The optimum value of ω is found to be 0.6. The yield of the desired product increases by about 13 % with the optimum value of $\omega = 0.6$ compared to the conventional isomerization reactor.

The appropriate thermal operating condition for the PSAR is isothermal condition. To approach the isothermal operating condition, the heat transfer in the PSA section is critical because it determines the uptake of the unreacted reactant in the reaction/adsorption step and the temperature of the effluent at the end of the PSA section in the desorption/reaction step. The developed non-isothermal PSAR model is therefore useful for the design, scale-up, and control and optimization purposes.

Abstrak tesis yang dikemukakan kepada Senat Universiti Putra Malaysia sebagai memenuhi keperluan untuk ijazah Master Sains

SIMULASI PENYERAP BUAIAN TEKANAN REAKOR UNTUK PENGISOMERAN N-PARAFIN

Oleh

LAI YIN LING

Oktober 2004

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Dalam tesis ini, satu matematik model untuk penyerap buaian tekanan-reaktor (PSAR) tak sesuhu untuk proses pengisomeran n-parafin telah dikembangkan. PSAR adalah suatu konsep baru yang menggabungkan proses pengisomeran paraffin biasa (n-parafin) dan pemisahan iso-parafin daripada campuran n/iso-parafin dengan meggunakan penjerapan buaian tekanan (PSA). Pengisomeran daripada n-pentana kepada iso-pentana telah digunakan untuk menjelaskan konsep baru ini. Turus PSAR itu dipadat dengan satu lapisan pemangkin (Y-zeolite) dan diikuti dengan satu lapisan bahan penjerap (zeolite 5A). Matematik model ini telah diselesaikan secara berangka dengan kaedah garis dimana persamaan perbezaan tertib kedua telah diturunkan kepada persamaan perbezaan tertib pertama. Kaedah penempatan bersama ortogon (OC) telah digunakan sebagai kaedah penurunan. Program komputer telah ditulis dalam FORTRAN 99.

Penyelesaian pengangkaan di dalam model PSAR ini telah disahkan dengan mengubahsuaikan nisbah panjang bahagian reactor kepada panjang kolum, ω. Apabila nilai bagi ω diubahsuaikan kepda nilai dekat 0, model PSAR akan dapat diturunkan kepada model PSA dan apabila diubahsuaikan kepada1, ia akan dapat diturunkan kepada model reaktor pada keadaan mantap. Nilai optima bagi ω ialah 0.6. Hasil produk yang terdapat dengan menggunakan PSAR ini telah meningkat sebanyak 13 % pada nilai optima $\omega = 0.6$ berbanding dengan reaktor pengiosmeran yang biasa.

Keadaan kendalian terma yang sesuai bagi PSAR adalah dalam keadaan sesuhu. Untuk mendekati keadaan sesuhu, pengaliran haba dalam bahagian PSA adalah penting kerana ia akan menentukan corong bahan tindak balas yang tidak bertindak balas dalam langkah tindak balas/penjerapan dan suhu bagi kumbah daripada bahagian PSA dalam langkah nyaherapan/tindak balas. Oleh yang demikian, model PSAR yang dikembangkan itu adalah berguna untuk reka ciptaan, pembesaran skala, kawalan dan pengoptimuman proses.

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I certify that an Examination Committee met on 15th October 2004 to conduct the final examination of Lai Yin Ling on his Master of Science thesis entitled "Simulation of Pressure Swing Adsorber Reactor for Isomerization of n-paraffins" in accordance with Universiti Pertanian Malaysia (Higher Degree) Act 1980 and Universiti Pertanian Malaysia (Higher Degree) Regulations 1981. The Committee recommends that the candidate be awarded the relevant degree. Members of the Examination Committee are as follows:

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This thesis submitted to the Senate of Universiti Putra Malaysia and has been accepted as fulfilment of the requirements for the degree of Master of Science. The members of the Supervisory Committee are as follows:

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DECLARATION

I hereby declare that the thesis is based on my original work except for quotations and citations which have been duly acknowledged. I also declare that it has not been previously or concurrently submitted for any other degree at UPM or other institutions.

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LAI YIN LING

Date:

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