A Review Paper on Design and simulation of tubular heat exchanging reactor for coupling exothermic and endothermic reactions

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Abstract - *Process intensification is the dramatic improvement in processing, substantially decreasing equipment size, energy consumption and waste production. Coupling or arranging two different reactions in chemical reactor reduces cost, increases efficiency, and reduces design complexities. Coupling exothermic with endothermic reactions together is proposed as a significant improvement in reactor performance, energy integration, size and area of the reactors. By combining endothermic and exothermic reactions in one reactor, a mutual utilization of thermal energy involved in reactions is expected to produce a saving energy and a cost-down for running in industrial reaction process. Double pipe heat exchanger is one type of tubular reactor suitable for such reaction coupling. In this work, heat exchanger is used as a plug flow model to analyse and compare the performance of co-current and counter-current heat exchanger reactors. Analysis is carried out for comparison of calculated results and simulated results. Practical analysis such as, exit conversion of the endothermic and exothermic reactions, the temperature peak (hot spot) of the exothermic reaction and the reactor volumetric productivity. Double pipe heat exchanger behaves like plug flow reactor, which are important for design, operational and control point of view, are presented.*

Key Words: **Coupling, exothermic and endothermic reaction, Counter-current and co-current heat exchanger reactors.**

1. INTRODUCTION

Reduction of equipment size, increasing the utilization of energy and reducing environmental impact these factors studied under process intensification and therefore has been widely studied. A novel reactor concept, which facilitates direct coupling of exothermic and endothermic reactions, is one example of process intensification which has attracted great attention. Since the exothermic and endothermic reactions take place simultaneously in the same heat exchanging tubular reactor, the equipment size can be markedly reduced and the utilization efficiency of energy and resources can be significantly improved. The simplest system involves an exothermic reaction and an endothermic reaction being run in counter current and co-current direction. A bi-directional fixed-bed reactor concept has also been developed. During the exothermic semi-cycle the fixed bed is heated and the stored heat is consumed in the next semi-cycle when the endothermic reaction takes place. In this system, however, the dynamic behavior of the reactor is complicated and inefficient heat integration can cause hot spots. In order to overcome these problems, a spatially segregated system that allows indirect heat exchange through a thermally conductive substrate has been proposed as an alternative. The exothermic and endothermic reactions take place in different parts of the system and the reactants can flow in co or counter-current manner in the reaction zones. Both tubular heat exchanging reactors and catalytic plate reactors (CPR) have been proposed. In the latter case, the catalysts for exothermic and endothermic reactions are loaded on opposite surfaces of a plate. The influences of varying wall thickness, thermal conductivity, catalyst loading, reaction temperature, and reactant composition and flow rates on the reactor behavior have been studied in detail by means of simulations. In most of the coupled systems which have been studied to date, the highly exothermic reactions involve combustion of hydrocarbons, with the endothermic reactions being reforming, cracking or dehydrogenation of hydrocarbons. Owing to thermodynamic and kinetic limitations, these strongly endothermic reactions have to be carried out at high temperature, which means that the reactors used in these systems must possess excellent heat transfer properties so that the heat absorbed in the endothermic reactions can be supplied efficiently. In the cases of conventional reactors placed in an oven, the reactions can be facilitated by direct heating. However, the equipment is complicated and the utilization efficiency of energy is very low. In recent years, monolith catalysts and reactors which use metallic monoliths as the support have attracted considerable attention. These catalysts and reactors have much better heat and mass transfer performance and much lower pressure drop compared with a conventional pellet-packed bed. They can also be constructed with a variety of flow channels and specific surface area according to the requirements of a given reaction system [1].

Highly endothermic heterogeneously catalyzed gas phase reactions at high temperatures with possible rapid but reversible catalyst deactivation are an industrially important class of chemical transformations. Examples of large industrial processes for this type of reactions are the dehydrogenation of lower paraffin's, the dehydrogenation of ethyl benzene and the production of synthesis gas. Processes for highly endothermic reactions with catalyst deactivation mainly in the method of energy supply for the endothermic reactions and the method of catalyst regeneration, predominantly determined by the catalyst properties and the rate of catalyst deactivation. Mixing endothermic reactants with exothermic reactants or other components, is termed as 'direct coupling', can eliminate the need for heat exchange and it can strongly reduce or completely avoid catalyst deactivation [3].

2. LITERATURE REVIEW

1. M. Bayat, M.R. Rahimpour

The author studied that the coupling of the energy intensive endothermic reaction systems with appropriate exothermic reactions reduces the size of the reactors and can improve the thermal efficiency of processes. One type of a suitable reactor for such a kind of coupling is the heat exchanger reactor. The catalytic methanol synthesis is coupled with the catalytic dehydrogenation of cyclohexane to benzene in an integrated reactor formed from two fixed beds separated by a wall where heat is transferred across the surface of the tube. A steady-state heterogeneous model of the two fixed beds predicts the performance of the two different configurations of the thermally coupled reactor. A co-current mode is investigated and the simulation results are compared with the corresponding predictions for the industrial methanol fixed bed reactor operating in the same feed conditions. The results of the study reveal that should the exothermic and endothermic reactions be located in the shell side and tube side, respectively, the methanol production rate will increase in comparison with the conventional methanol synthesis reactor as well as the case where the exothermic reaction is located in the tube side and endothermic reaction in the shell side.

1)Concluding Remark- The methanol synthesis reaction, which was coupled with the dehydrogenation of cyclohexane to benzene using indirect heat transfer in a catalytic heat-exchanger reactor, was studied for two different configurations by a one dimensional model. The reactors consist of two separate sides for exothermic and endothermic reactions. In this study, the dehydrogenation of cyclohexane to benzene was used to consume the generated heat from the methanol synthesis. This is similar to the temperature profile along the tube filled with catalysts within the methanol conventional reactor. The simulation results show that there is extremely favorable profile of temperature in exothermic side of proposed configuration of TCR and represent 6.55 and 10.5% enhancement in the methanol production in comparison with CR and CTCR, respectively.

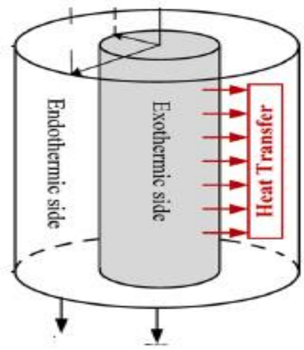

Fig1. Thermally coupled reactor

2. R.C. Ramaswamy

Author studied that the reactions couplings reduces equipment size, increases utilization of energy in a single reactor system. There are many types of reactor for coupling exothermic and endothermic reactions but a reactor suitable for such coupling is the heat exchanger reactor. Author in this work reported same phase plug flow reactor set up which is used to analyze and compare the performance of co-current and counter-current heat exchanger reactors. A parametric analysis is carried out to address the vital issues, such as the exit conversion of the endothermic reaction, the temperature peak (hot spot) of the exothermic reaction and the reactor volumetric productivity. The measures to reduce hot spots by different catalyst profiling techniques are also addressed. Some features of the dynamic behavior exhibited by these reactors, which are important from design, operational and control point of view, are presented.

2) Concluding Remark – The behavior of counter-current and co-current heat exchanger reactors coupling exothermic and endothermic reactions are analyzed using plug flow reactor set up. In general, the heat exchanger reactors yield higher exit conversion for the endothermic reaction than the adiabatic reactor. The temperature peak on the exothermic side is lower in co-current reactor than that in the counter-current reactor. The hotspot on the exothermic side is a major concern in these reactors and we observed that these hot-spots could be reduced drastically by suitable catalyst activity profiling in the co-current reactors. Observing profiles of performance, the reaction front spreads over the reactor providing a more uniform heat source to the endothermic side. However, during the transient mode of operation the temperature peaks on the exothermic side exceed the steady state temperature peak. This may have adverse impact on the catalyst used.

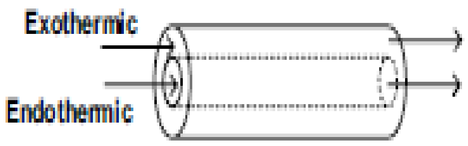

Fig 2. Adiabatic coupled reactor

3. Amina M. Bruschi

Author reported that the steam reforming of ethanol is carried out in a microreactor for hydrogen production. The heat for the endothermic reactions is supplied by means of ethanol combustion in air, which is carried out in contiguous microchannels. The same Palladium based catalyst is assumed to be coated on both reforming and combustion channels. By means of a 1D heterogeneous mathematical model, the influence of the feed temperatures of both streams on the reactor performance is analyzed. The results concluded that the degree of preheating of both streams has a strong influence on the hydrogen yields and maximum temperatures. The effect of the flow rate and composition of the fuel stream on the hydrogen yields is also studied. Fairly high hydrogen yields were obtained with low methane slips, within a feasible range of temperatures for the Pd catalyst to avoid catalyst deactivation. These maximum temperatures could still be further reduced by means of an optimal selection of the air flow rate and ethanol molar fraction on the fuel side, or using distributed feed of fuel along the reactor length.

3) Concluding Remark - The appropriate preheating of both process streams, together with adequate values of flow rate and ethanol molar fraction in the feed of the combustion side, are the keys to reach high production rates. If the operating conditions are correctly selected, the reactor will be ignited close to the entrance and high temperatures along the reactor length will take place, leading to low methane slips and high hydrogen yields.

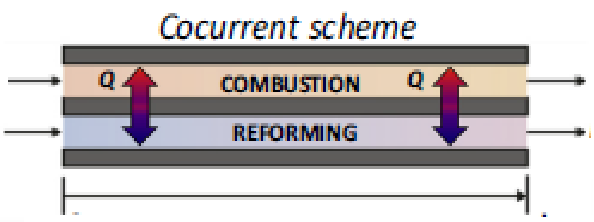

Fig 3. Simulated reformer

4. Akira Igarashi

By combining endothermic and exothermic reactions in one reactor, a mutual utilization of thermal energy involved in reactions is expected to produce a saving energy and a cost-down for running in industrial reaction process. In this case, a wall-type reaction system is thought to be suitable because such reaction system is good at exchangeability of thermal energy by conductive heat transfer. This study supposed a wall-type reaction system consisting of endothermic and exothermic reaction channels stacked up and a fixed-bed reaction system of the same configuration, and compared them by numerical simulation in the case where endothermic and exothermic reactions progress simultaneously. In the fixed-bed reaction system, heat transfer in the catalyst bed takes place by convection, and this transfer becomes the rate-limiting process. Accordingly, occurrence of hot spot in the exothermic channel and shortage of thermal energy in the endothermic channel were predicted. This trend became distinct by making the feed gas directions flowing in the two channels countercurrent and by stacking the channels in multiple tiers. In the wall-type reaction system, however, the temperature distributions in the exothermic and endothermic channels almost conformed to the set temperatures, and the temperature difference between channels was small. Even if the feed gases flowed in countercurrent and even if the channels were stacked several deep, this trend did not change. In the wall-type reaction system, the exchange of thermal energy would take place efficiently by conductive heat transfer between the endothermic and exothermic channels. Furthermore, it was inferred that the wall-type reaction system would provide a stable operation in mutual utilization of thermal energy.

4) Concluding Remark - Performances of the wall-type reaction system with exothermic and endothermic reaction channels stacked singly and alternately were numerically investigated, comparing them with that of a fixed-bed reaction system with the same configuration. The simulated temperature profiles in the fixed-bed reaction system predicted a hardly controlling the system, for generating a large difference in temperature. Such tendency was accelerated by the deeply stacking and in the countercurrent flow direction off feed.

5. P.A. Ramachandran

Author reported that the steady state and the dynamic behavior of coupling exothermic and endothermic reactions in directly coupled adiabatic packed bed reactors (DCAR) are analyzed using one-dimensional pseudo-homogeneous plug flow model. Two different configurations of DCAR (simultaneous DCAR—SIMDCAR and sequential DCAR—SEQDCAR) are investigated. In SIMDCAR, the catalyst bed favors both exothermic and endothermic reactions and both reactions occur simultaneously. SEQDCAR has alternating layers of catalyst beds for exothermic and endothermic reactions and hence the exothermic and endothermic reactions occur in a sequential fashion. The performance of both reactors, in terms of conversion achieved and manifested hot spot behavior, is compared with that of the co-current heat exchanger type reactor. Various possible operational regimes in SIMDCAR have been classified and the conditions for the existence of hot spots or cold spots in SIMDCAR are obtained analytically for the first order reactions with equal activation energies. The reactor behavior for the reactions with non-equal activation energies is also presented. The preliminary criteria for the selection of suitable reactor type and the general bounds on the reaction parameters to obtain the desired conversion for endothermic reaction with minimal temperature rise are proposed. The dynamic behavior of these reactors is important for control applications and we have reported some of the transient behavior.

5) Concluding Remark - This work investigated the different modes of conducting exothermic and endothermic reactions in directly coupled adiabatic reactors and the reactor performance is compared with that of the co-current reactor. The conditions for the existence of hot spot or cold spot are presented. The direct coupled adiabatic reactor exhibits a huge range of temperature profile patterns based on the relative magnitudes of the heat generation rate and the heat consumption rate. Thus, it can behave as an isothermal reactor, an exothermic or an endothermic reactor or the reactor where the endothermic reaction follows the exothermic reaction or the exothermic reaction follows the endothermic reaction.

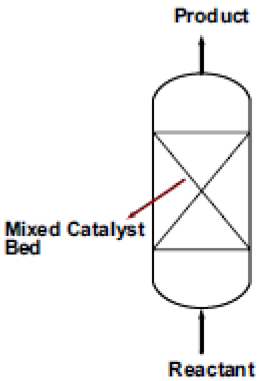

Fig 4. Coupling in packed bed reactor

6. M. van Sint Annaland

Author studied the new concept of reactor which is studied for endothermic heterogeneous catalyzed gas phase reactions which is highly exothermic at high temperatures with rapid but reversible catalyst deactivation. The reactor concept aims to achieve an indirect coupling of energy necessary for endothermic reactions and energy released by exothermic reactions, without mixing of the endothermic and exothermic reactants, in closed-loop reverse flow operation. Periodic gas flow reversal incorporates regenerative heat exchange inside the reactor. The reactor concept is studied for the coupling between the non-oxidative propane dehydrogenation and methane combustion over a monolithic catalyst. Two different reactor configurations are considered that are sequential reactor configuration, where the endothermic and exothermic reactants are fed sequentially to the same catalyst bed acting as an energy repository and the simultaneous reactor configuration, where the endothermic and exothermic reactants are fed continuously to two different compartments directly exchanging energy. The dynamic reactor behavior is studied by detailed simulation for both reactor configuration. Energy constraints, relating the endothermic and exothermic operating conditions, to achieve a cyclic steady state are discussed. Furthermore, it is indicated how the operating conditions should be matched in order to control the maximum temperature. Also, it is shown that for a single first order exothermic reaction the maximum dimensionless temperature in reverse flow reactors depends on a single dimensionless number.

6) Concluding Remark - A new reactor concept for highly endothermic reactions at high temperatures with possible rapid but reversible catalyst deactivation based on the indirect coupling between endothermic and exothermic reactions and the reverse flow concept has been studied. Two different reactor configurations have been considered: the sequential reactor configurations and the simultaneous reactor configurations in co-current and counter-current operation mode. In the sequential reactor configurations, the endothermic and exothermic reactants are fed discontinuously and sequentially to the same catalyst bed acting as an energy repository. In the simultaneous reactor configurations the endothermic and exothermic reactants are fed continuously to two di9erent compartments exchanging energy. Their reactor behavior has been investigated via detailed numerical simulations.

7. Grigorios Kolios

Author studied that the autothermal multifunctional reactor is a novel and new concept in process integration and intensification. They can be implemented as a countercurrent or reverse-flow reactor. A promising field of application is the coupling of endothermic and exothermic reactions. Methane steam reforming coupled with methane combustion is considered as a particular example. Various types of novel and new reactor configurations with co-current and counter current flow in the reaction zone will be discussed by evaluating a numerical simulation and an example for experimental verification will be presented.

7) Concluding Remark - Maximum temperature control is the key issue in coupling endothermic and exothermic reactions in an autothermal mode of operation. For comprehensive analysis of different design alternatives a staged approach is necessary which includes models of different levels of complexity along with appropriate analytical and computational methods. Based upon such an approach, it was possible to establish the desired operating conditions in a wall reactor with the asymmetric countercurrent operation mode. However, this leads to a highly sensitive state of operation. A modified design employing co-current heat exchange in the catalytic part combined with countercurrent end sections extends the limits of the optimal operating regime substantially.

3. CONCLUSIONS

Review of reactions couplings using different reactors and configuration with simulation were discussed in the paper. Many experimental and modelling studies have been presented which shows effective use of reaction couplings. Process intensification in the chemical industries is the novel concept which reduces size and area of the chemical plants. Coupling of exothermic and endothermic reactions is one of them. There are many ways to couple the different types of chemical reactions in a single tubular reactor, but the tubular adiabatic reactor coupling gives better result. In this reactor system no energy loss from the system and no energy gain by the system. This adiabatic nature of the reactor utilizes maximum amount of energy produced from exothermic reaction. Also this reaction coupling is directly depends upon heat of the reactions which we are going to use in the reactor system. Selection of reactor configuration i.e. co-current or counter direction coupling is most challenging part so as to achive the maximum conversion of reactants. Using co-current configuration in adiabatic reactor gives better result and conversion of reactants is maximum. Simulation of these reactors will be carried out to compare the results in order to get optimum conversion. Temperature in this reactor is at maximum peak point so it increases rate of reactions. From all this studies it can be seen that the utilization of adiabatic reactor with co-current configuration shows successful and promising results and further it can be useful element for chemical industries.

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