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Conceptual foundations of chemical kinetic modeling

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Chemical engineers (primarily) and also other discipline engineers with a background in chemistry who have a need to understand the basic steps and concepts upon which the assembly of complex Detailed Chemical Kinetics Models (DCKM) were found. The aim is for the DCKM to become part of a chemical reactor model of a given physical configuration and size in order to make predictions of reactor performance and trace contaminant formation. The following topics are to be discussed in the presentation: (1) The fundamental steps in the assembly of complex chemical kinetic models composed of hundreds of elementary reaction; (2) Guidelines on how to generate the chemistry which is part of the DCKM, the most important consideration without the proper chemical steps, the final reactor modeling is useless as a predictive tool of reactor performance; (3) It is also necessary to present how to generate the thermo-chemical data for the reactions as well as chemical kinetic coefficients since these are a necessary data for reactor modeling; (4) Basic concepts of modern Computational Chemistry are introduced since it is a tool used to generate thermo-chemical data and reaction rate coefficients for elementary reactions. Most often experimental data is lacking or difficult to obtain; (5) Concepts of chemical kinetic model validation (independent of reactor size or configuration) as well as chemical reactor scale-up are also introduced; (6) Examples are provided for the development of combustion mechanisms for two simple fuels (methane, hydrogen sulfide) and a CVD catalyzed reaction.

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Volume loss modeling for lost circulation, Hartha formation, South Rumalia Field, Iraq

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Development of producing reservoirs using horizontal wells is now common in primary, secondary and tertiary oil recovery processes. However in Kuwait, most of the existing wells are vertical wells and at the same time there are several reservoirs in which horizontal wells could significantly improve the oil production. Because of the large surface area associated with them, the production of oil by horizontal wells can be very efficient. In fact, the performance of horizontal wells can reach an order of magnitude higher than that of vertical wells. However, reservoir heterogeneity and the existence of fractures can conspire to make the production process less efficient. Therefore, there should be a need for a comprehensive understanding of the performance behavior of horizontal wells before they are tried in the field. This study discusses the steps undertaken to develop and evaluate a small-scale simulation model of a candidate reservoir in order to investigate the benefit if/any of using horizontal wells as a new production strategy. A systematic approach was followed to design and study the performance of several scenarios in order to recommend future management and production strategies under which the use of horizontal wells in this reservoir may yield better recovery. Sensitivity analysis of horizontal well length, well location, orientation and well completion on the reservoir performance were investigated. In each case, the reservoir performance using horizontal wells was compared to that of using vertical well. This study has resulted in significant new insights into the performance of horizontal well in this reservoir. Results from this study show that the use of horizontal wells is a very attractive management strategy even with a short lateral horizontal well length. An optimum horizontal well configuration was obtained that includes well location, orientation, lateral horizontal well length and the penetrated layers.

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