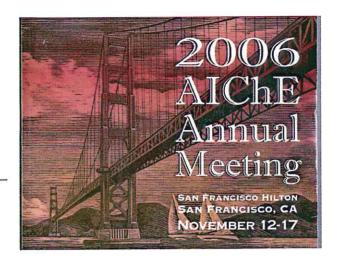
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Complete Abstract(s)

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Formulation and Validation of Bivariate Population Balance Models

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Mathematical Modelling of Nano-Particle Formation and Evolution in Combustion Processes Alessandro Zucca, <u>Daniele L. Marchisio</u>, Antonello A. Barresi and Giancarlo Baldi

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Design and Scale-up of Chemical Reactors for Nanoparticle Precipitation Emmanuela Gavi, <u>Daniele L. Marchisio</u>, Antonello A. Barresi and Giancarlo Baldi

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Comparison of the Performance of a Reverse Flow Reactor and Networks of Non-Stationary Catalytic Reactors for Catalytic Combustion of Methane in Lean Mixtures

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Although the operation under unsteady state is generally avoided and continuous operation is preferred in the chemical chemical industry, this mode of operation can often lead to a better performance. Because of this, forced unsteady state reactors are object of increasing interest. n particular, the systems based on the periodic reversal of the feed flow direction, called reverse flow reactors (RFR), and the reactor networks of two (RN2) or three reactors (RN3) in series where the feed position is periodically changed from a reactor to the following one in the sequence seem to be particularly promising.

The simple operation procedure of the RFR leads to important advantages in some catalytic processes. So, reverse flow operation is particularly advantageous in the case of the catalytic combustion of lean air-hydrocarbons mixtures, mainly due to its high thermal efficiency. This technology has been implemented industrially for the abatement of VOCs, and the research on this field is still very active. One of the main drawbacks of this technology is the by-pass of relatively large amounts of unconverted hydrocarbons when the flow direction is reversed.

Unsteady reactor network consists of a series of fixed bed reactors connected in a closed sequence with periodical variations of the feed position. Contrary to the RFR, the flow direction is maintained in this device. This fact has two important advantages: ensure a uniform catalyst utilization and avoid the presence of unconverted gas by-pass.

The scope of the present work was to compare, for similar operation conditions, the performance of a RFR and RN of two and three reactors. Different CH4/air mixtures of 0.1-1 % were selected as feed for the combustors. Adiabatic bench-scale reactors (30 cm length, and 14 mm inside diameter) and a commercial Pd/Al2O3 catalyst (dp=0.7 mm, k0=1.625•108 s-1, Ea=9.124•104 J/mol) were considered for these studies. Reactor behaviour (considering as adiabatic) was simulated using a heterogeneous unidimensional model in all the cases. Model was experimentally validated for the RFR operation in the experimental rig described in the literature1.

In order to characterise the performance of these devices it is important to study the influence of the main operating conditions, namely inlet temperature, flow rate and composition, as well as the switching time (i.e. the time interval occurring between two successive changes of the feed position), on the stability of the reactor, in order to find the values (or range of values) of these variables that ensure autothermal behaviour. Beside this, the influence of these variables on the maximum temperature that can be reached in the reactor has to be pointed out in order to avoid catalyst overheating and deactivation.

In the case of RFR, there is only one range of values of the switching time that ensures stable operation, being the reactor extinct for switching times higher than 1100 s (working with 0.1 % of methane), 18000 s (working with 0.5 % of methane) and 2450 s (working with 1 % of methane), respectively. The situation is quite different working with RN. For these configurations, the presence of different interval of values of the switching time where the reactor can be operated safely (some of them very narrow) has been observed. As general trend, these intervals have been found both working at low switching times (50-500 s for RN2) and high switching times (750-1400 s for RN2 and 472-850 s for RN3). For reactor networks of three reactors the low switching time stability interval is only observed with concentrated streams (1%), whereas for networks of two reactors, both intervals are observed for all the methane concentrations studied. The width of the intervals (a key issue for control purposes) is higher for the network of two reactors and for a given network, this width increasing as the concentration of methane increases.

Concerning to the evolution of the catalytic bed temperature, it increases as the concentration of methane increases for all the configuration studies (as expected), but the behaviour is quite different depending on the concentration studied. So, for the most concentrated feed, the maximum temperature found in the RFR is always higher than the corresponding to reactor networks, whereas for lower methane concentrations, maximum temperatures are higher for the reactor networks, especially when working in the high-switching time interval. An important difference between RFR and RN is that the evolution of the maximum temperature with both time (in a given experiment) and switching time (comparing different experiments) is sharper for RN whereas is smoother for RFR. This means that the catalyst used in RN suffer strong more marked temperature variation, which can also affect to the catalytic properties.

The reported work suggests that, considering both the stability intervals and the temperature profiles inside the reactor, RFR is a better choice for the treatment of hydrocarbon-air lean mixtures.

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