Various types of models

Industrial processes and scale-up
Lesson #2

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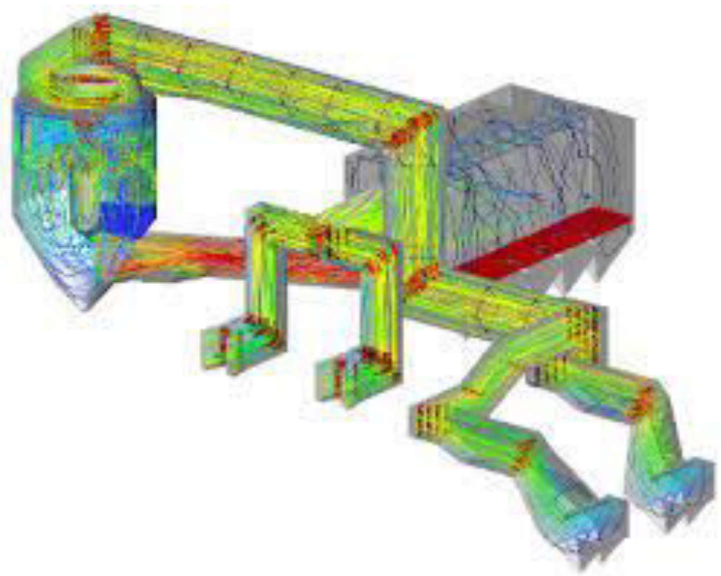
Representation by means of models is a fundamental operation in scale-up study.

A model can be DEFINED as the approximate representation of a process, mechanism or phenomena.



Three major classes of models:

1) Mathematical models
2) Physical models
3) Chemical models

Models have the **following aims**:

- To represent and condense the data by using known basic equations
- Separation of the essential from the accessory, simplification, clarification, identification of controlling mechanism
- Forecasting the bahavior of the system in the investigated domain of plant conditions
- Development of an optimal control system for a given operation
- Training in running production units

1) Different form of Mathamatical Models

A mathematical model can assume different forms according to its level of description:

1.1) Fundamental model and formal model
1.2) Simple model and compex model
1.3) Stady-state and dynamic models
1.4) Deterministic and probabilistic models

1.1) Fundamental model and formal model

The **fundamental model**, called also «representation model», «knowledge model» or «phenomenological model», is DEFINED as a set of equations mainly related to the description in time and in space:

- of mass and energy balance compiled on the different compounds of an ELEMENTARY CELL with given contours
- of mass, heat and momentum transfers and electric charge.

These equations developed for an elementary cell are then extended to the whole space of the process.

1.1) Fundamental model and formal model

The less ambitious **formal model** is aimed to describe EMPIRICAL CORRELATIONS between variable and response in form of algebric equations.

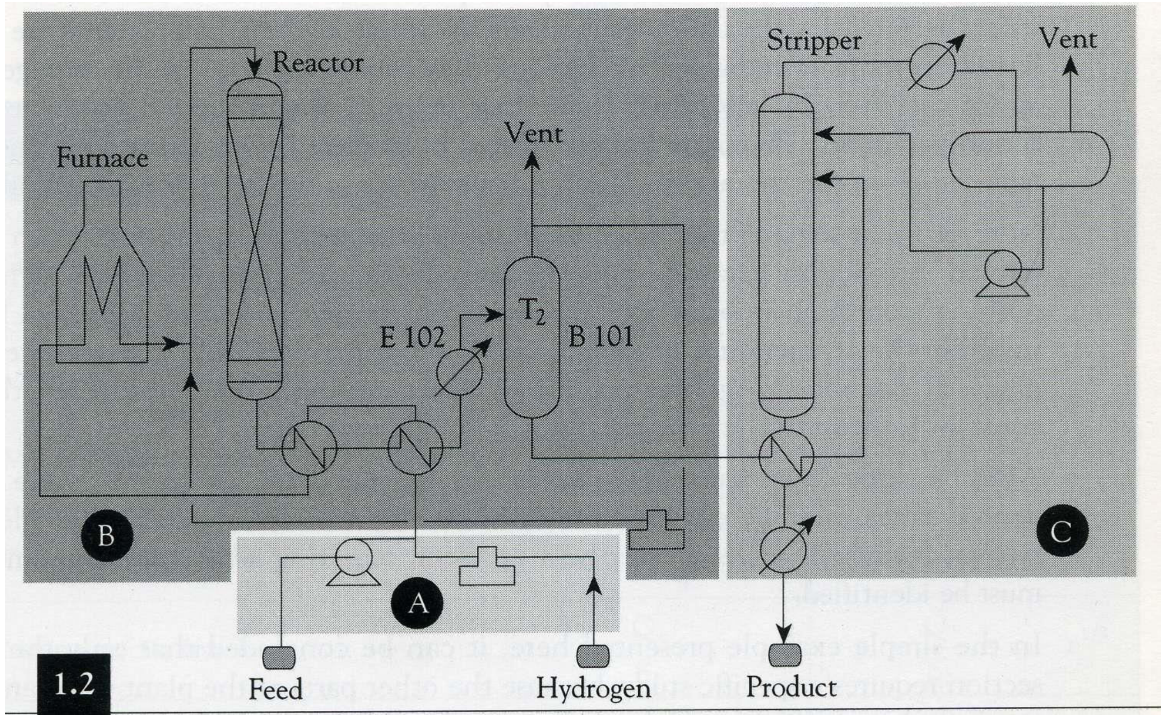
This kind of model provide NO EXPLANATION of a phenomenological nature.

The easiest example can be an interpolation of experimental data.

1.2) Simple model and complex model

In a given installation, the behavior of each piece of equipment can be described, in general, by a simple model. However, the different components quite never operate in isolation, interacting among them.

The COMPLEX MODEL is made up of all the specific simple models, combined with input and output conditions for each of the interconnected parts.



This system can be divided into three indipendent sub-system. System B, which includes a recycle, CAN NOT BE BROKEN DOWN FURTHER and it contains several parts with disctint functions. IT CAN BE DESCRIBED BY A COMPLEX MODEL.
The models of sub-systems A and C are simple.
These defintions are not very rigorouses.

1.3) Steady-state model and dynamic model

The **steady-state model** refers to steady-state conditions, that means that the values of the variables having been fixed, the system has responded by shifting towards a STATE OF EQUILIBRIUM, AND THIS STATE IS EXAMINED WITHOUT BEING CONCERNED WITH THE WAY IN WHICH THIS STATE HAS BEEN REACHED.

The system is PHOTOGRAPHED AT DIFFERENT TIME INTERVAL. This in a key point: the time is a variable, but considering all the system in fixed condition; for example in one reactor there is a reaction with its kinetic behavior, but the time space required to bring the system to the fixed temperature and pressure condition is not considered.

Commercial software example: PRO II

1.3) Steady-state model and dynamic model

A **DYNAMIC MODEL** (unsteady-state) is encountered:

- In batch operations in which the values of the variable change constantly over time
- In continuous operations in a transient phase of start-up, altered condition or shut-down
- In continuous operation in which certain variable are subjet to disturbances such that the system never reaches its stable position

Commercial software example: DINSYM (Dinamic Symulation): there is the date and the clock!

1.3) Steady-state model and dynamic model

Intermediate case between these two models may exist, for example when a slow drift is observed in the equilibrium position. This situation is often present in industrial plant using catalysts, which presents progressive deactiviation. In this case, it is useful to consider the real model as a succession of several steady-state models for the differnt cycle (start, middle and end of cycle).

The analysis of synamic models is very important for the design of a monitoring/control system for the process, especially if the process has a tendency to runaways.

1.3) Steady-state model and dynamic model

Summarizing, for a given set of variables:

- the STATIC MODEL serves to describe the situation which should be established more or less rapidly.

- The DYNAMIC MODEL allows a description of the unsteady-state periods in approaching this state of equilibrium

1.4) Deterministic model and Probabilistic model

All the model discussed observed the PRINCIPLE OF DETERMINISM: «any given cause will always have the same effect».

A probabilistic model is based on a different principle, baed on the idea that only overall forecastes, of a statistical nature, can be formulated («Stochaistic approach»).
Examples include the dendritic crystal growth, the path followed by liquid streams on surface and in granular materials, the sol/gel transition in macromolecules…..

Whenever it is possible to describe a process by considering probabilities of existence or collision or preferential passage, it is advantageous to use probabilistic models, also if the model can only give average values.

Prerequisites for constructing a mathematical model

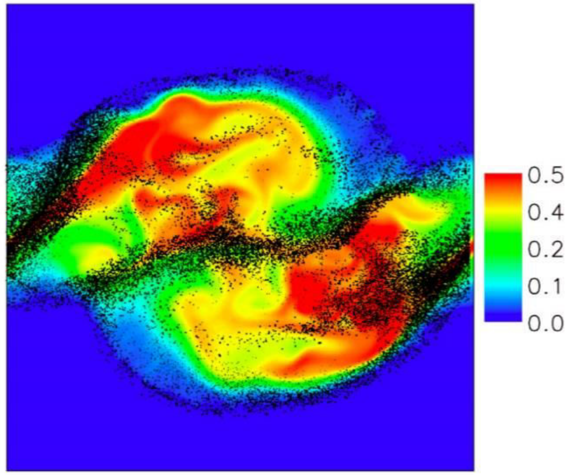
The construction of a good mathematical model requires the availability of reliable data and results. These data and results must be obtained in conditions of good reproducibility, diversity and representativity and must be based on sensors (compositions, flows, temperature…) which are carefully selectely and positionated on the plant.

The repetition of the base experiment is mandatory for:

- **Quantify the probable errors**
- **Validate (or invalidate) imagined models**
- **Discriminate between several possible models**
- **Verufy the coherence of all the balances**

IT IS TOTALLY ILLUSORY TO ATTEMPT TO VALIDATE A SOPHISTICATED MODEL IN THE ABSENCE OF AN ADEQUATE BODY OF RELIABLE RESULTS.

Physical models



Mixture fraction and droplets distribution

Physical models are based on a concrete support: the mock-up.

Physical models supplement mathematical models in two ways:

1) **They provide qualitative data qhich can be translated in terms of design**
2) **They help to collect quantified data, indispensable for mathematical treatement**

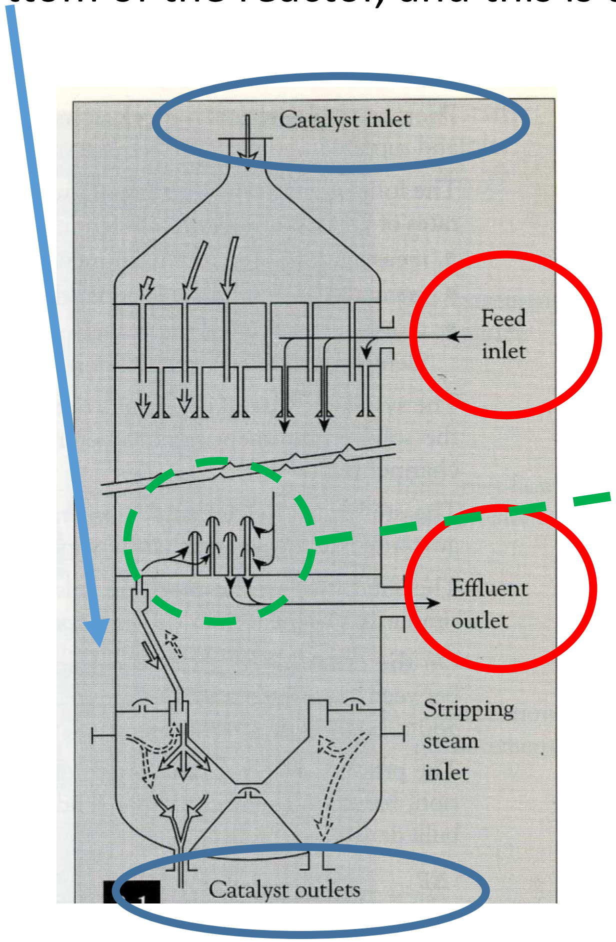
The use of physical models is recommended when the operation is liable to involve problems of TRANSFER, DIFFUSION, DISPERSION AND FLOW, maybe connected with THERMAL EFFECTS.

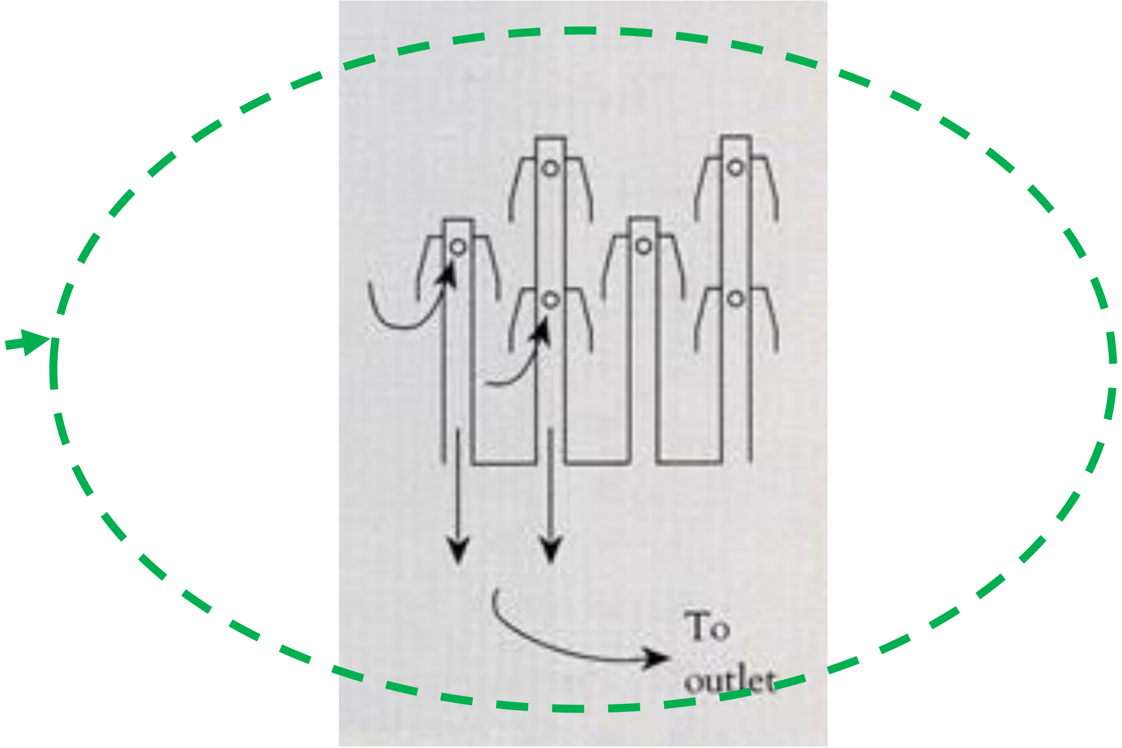
Actually, every operation involving at least two phases incorporates all these factors, and this is sometime true even with a single phase!

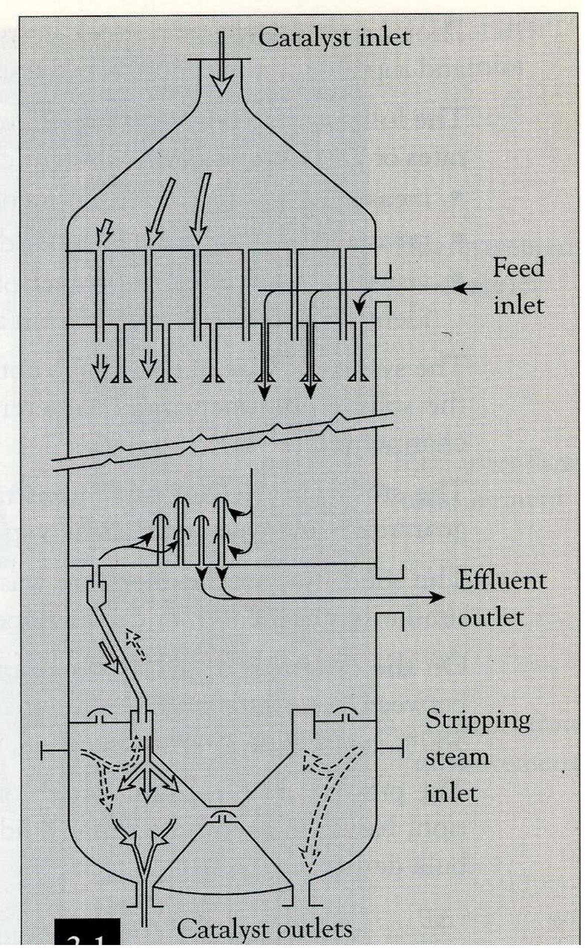
Physical models: example

«Determination of the maximum permissible velocity for the disengagement of the effluent vapors in a downward cocurrent moving bed»

In the downwards cocurrent moving beds, the effluent gas must be separated from the solid at the bottom of the reactor, and this is done by disengagement channels like those swohwn in the figures

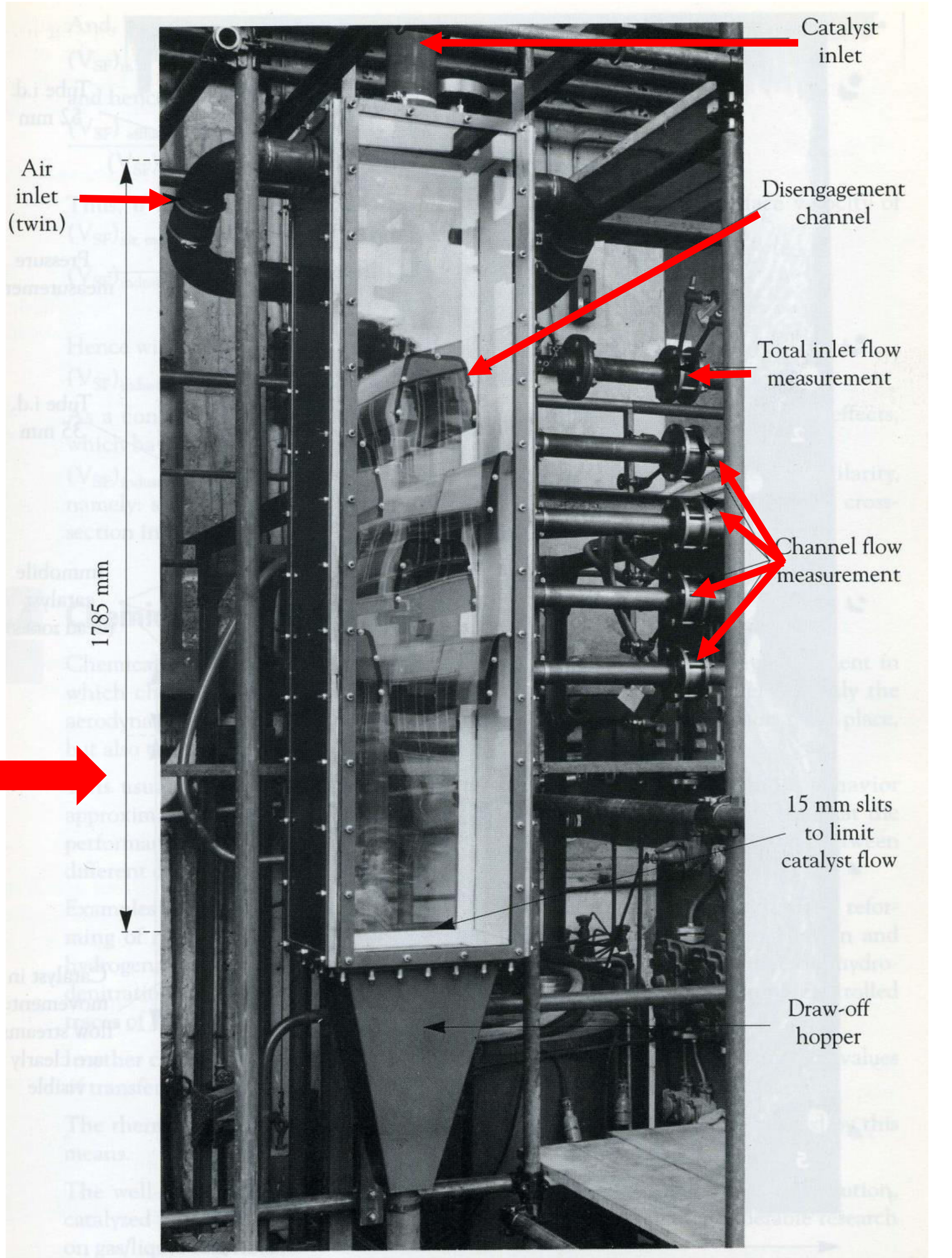






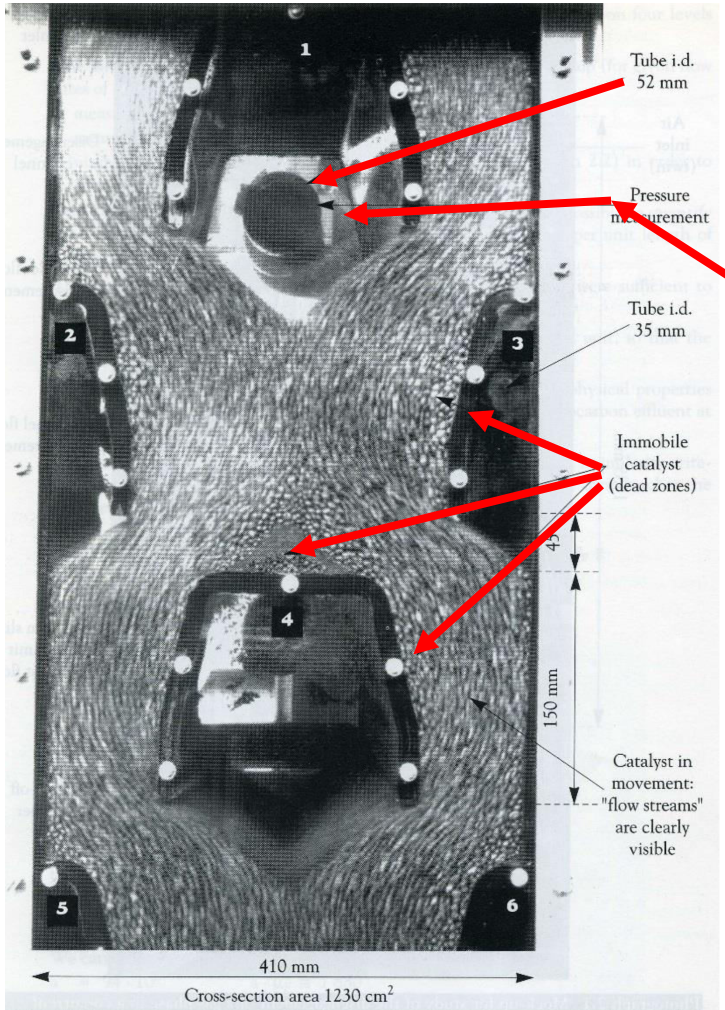
If the speed passage of the gas into the channel becomes excessive, this causes the antrainment of the solid with the reactor effluent. To prevent this situation, it is mantain this speed limit beyond a certain limit.

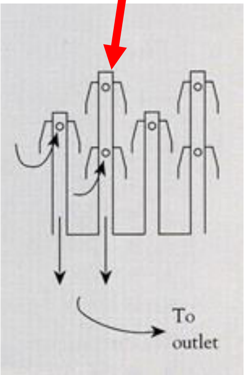
It is easy to determine this threshold by using a mock-up which replicates the geometric confermation of the channels.



Information obtained by mock-up experiment:

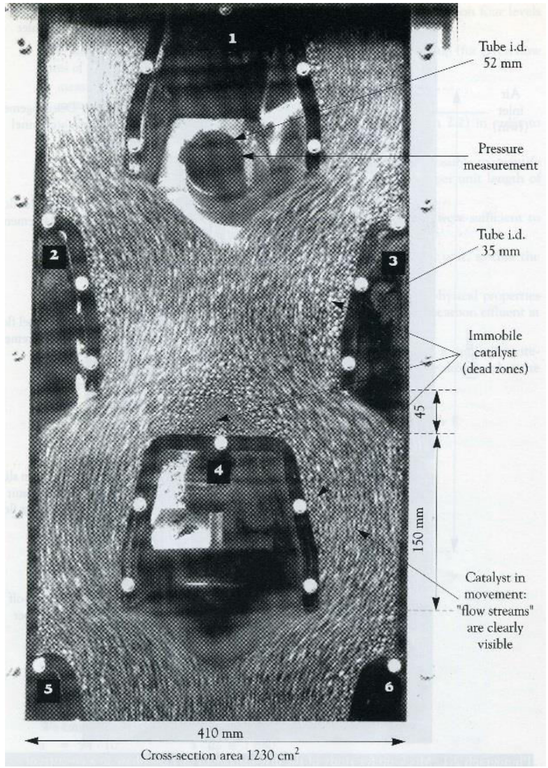
- Measure of solid entrainment in the different elements
- Measure of pressure under the caps of the different channels
- Visual inspection of the travel of the catalyst beads in order to identify dead zones, acceleration zones and voids.





The mock-up experiments allowed to:

- Quantify the solid entrainment, by determining a maximum air flow rate per unit lenght of channel in $\frac{kg}{s\,m}$
- Demonstrate that two stage of channel were sufficient to guarantee disengagement of the vapors.



The solid used in the mock-up experimenta was the solid used in the industrial unit: no problem

BUT

It was necessary to account for differences in physical properties between the simulated fluid (air at 20°C) and the actual fluid (hydrocarbon effluent at 380°C).

Calculation of the surface velocity (V_{SF}) in plant condition (hydrocarbon effluent @ 380°C)

From the theory, the following equation can be used:

$$\frac{(V_{SF})_{effluent,industrial\ unit}}{(V_{SF})_{air,mock\ up}} = \left(\frac{\rho_{air}}{\rho_{eff}}\right)^{1/2}$$

Now, if the mock-up displays incipient solid entrainment at a surface velocity of $(V_{SF})_{air,mock\ up}$ entrainment will be observed in the industrial unit for:

$$(V_{SF})_{effluent,industrial\ unit} = (V_{SF})_{air,mock\ up}\left(\frac{\rho_{air}}{\rho_{eff}}\right)^{1/2}$$

Being: $\rho_{air} = 1.28\,\frac{kg}{m^3}$ and $\rho_{eff} = 0.98\,\frac{kg}{m^3}$

$$\boldsymbol{(V_{SF})_{effluent,industrial\ unit} = (V_{SF})_{air,mock\ up} \cdot 1.14}$$

$$(V_{SF})_{effluent,industrial\ unit} = (V_{SF})_{air,mock\ up} \cdot 1.14$$

Now, be carefully!

Considering CONSERVATIVE MEASURE (we want to be absolutely sure) and taking into account of possible wall effect on the reactor, it is convenient to use:

$$(V_{SF})_{effluent,industrial\ unit} = (V_{SF})_{air,mock\ up}$$

This study and this calculation are correct only if we respect the geometric similarity: same ratio between disengagement passage cross section and passage cross section in the bed, and same number of level

Chemical models

Chemical models are used in chemical reactors, where chemical transformation take place. In this case we have to model not only the aerodynamic and hydrodynamic conditions in which the reaction takes places, but also the transformation itself.

The application of chemical models allows both a rigorous investigation of the reaction process involved (basic research) and the collection of quantified data useful in design the chemical reactor (applied research).

Chemical models, i.e. TEST REACTIONS

The basic idea of chemical models:

In chemical models we use reactions involving a SPECIFIC COMPOUND WHOSE BEHAVIOR APPROXIMATES THE AVERAGE BEHAVIOR OF A FAMILY OF COMPOUNDS.

Some examples:

- Catalytic cracking of cumene
- Catalytic reforming of n-Heptane
- Hydrogenation of benzene

Chemical models, i.e. TEST REACTIONS

The performance obtained during the TEST REACTIONS serves:

1) TO MAKE COMPARISONS between different catalysts or different combinations of operating conditions.
2) to obtain numerical value of transfer parameters (for example interfacial area, mass and heat transfer coefficient…)
3) To investigate thermal effect of the reaction

As industrial example of chemical models, the reaction of oxidation of sulfite by air in aqueous solution, catalyzed by cobalt ions, has facilitated considerable researches on gas/liquid reactions.

Chemical models, i.e. TEST REACTIONS

Chemicals model are useful to simplify the overall approach to the mechanism, by highlighting the major features of the transformation and the presumed relative importance of the different factors involved: chemical kinetics, more or less disturbed by transfer limitations.

Valuable information can be obtained on the location of the reactio and the limitative steps of the process.

<u>This study are facilitated because by chemical model it is possible identify model molecule instead of complex sets for which a detailed analysis is impossible</u>

Final remarks

<u>THE DISTINCTION BETWEEN MATHEMATICAL, PHYSICAL AND CHEMICAL MODEL REMAINS FORMAL!!!!!</u>

The harmonious combination and choice of the models to be used are the duty of the experimental worker. There are not strict rules, except the funfamental:

It is illusory to attempt to construct a sophisticated mathematical model, if suitable experimentation does not help to validate it within reasonable limits of time and cost.