FOUR MODELS FOR THERMO-CHEMICAL SIMULATIONS OF INDUSTRIAL FURNACES

by

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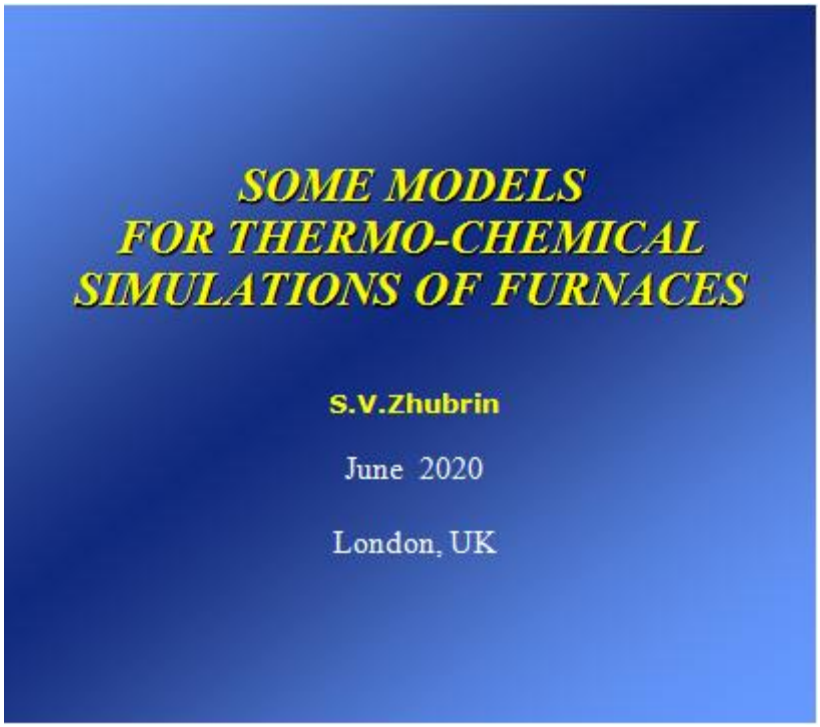


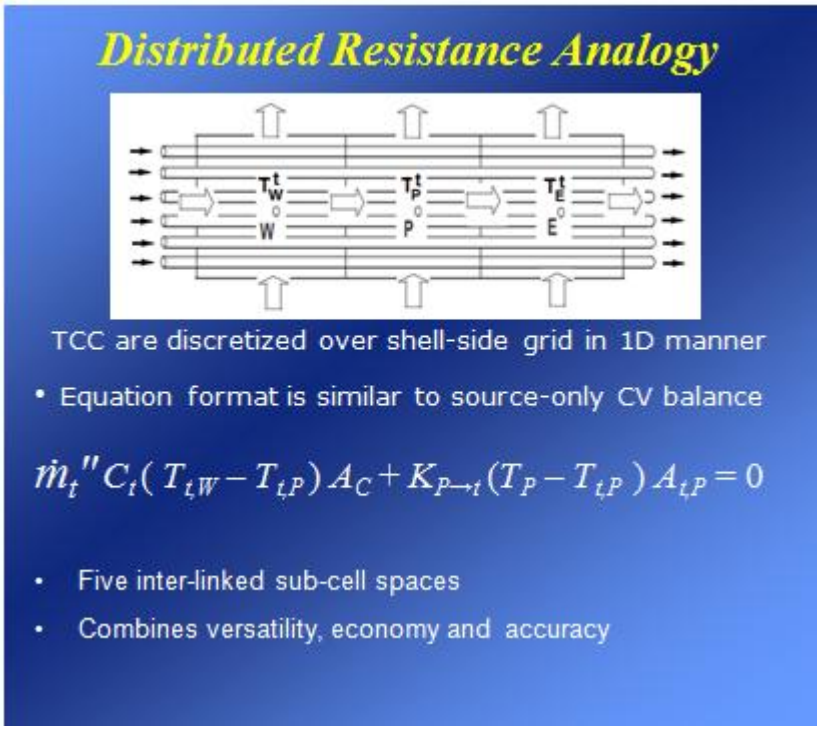
This presentation has been designed for the participants of the meeting with personnel of CIVS of Purdue University (USA) and ACFDA (Canada) held on-line on 24th of June 2020.

Special attention is given to four models referred below as DRA, DRM, SRM and D-CASE. They have been selected as most interesting to CIVS during preliminary discussions of potential collaborative projects. All of those present can be expected to be familiar with the nature of the models through either their own experience or by the documents disseminated before meeting. Therefore only a brief overview of key points for each model will be provided and references to the sources of additional information will be cited where appropriate.

A few years back we have come across very interesting and challenging project [1].

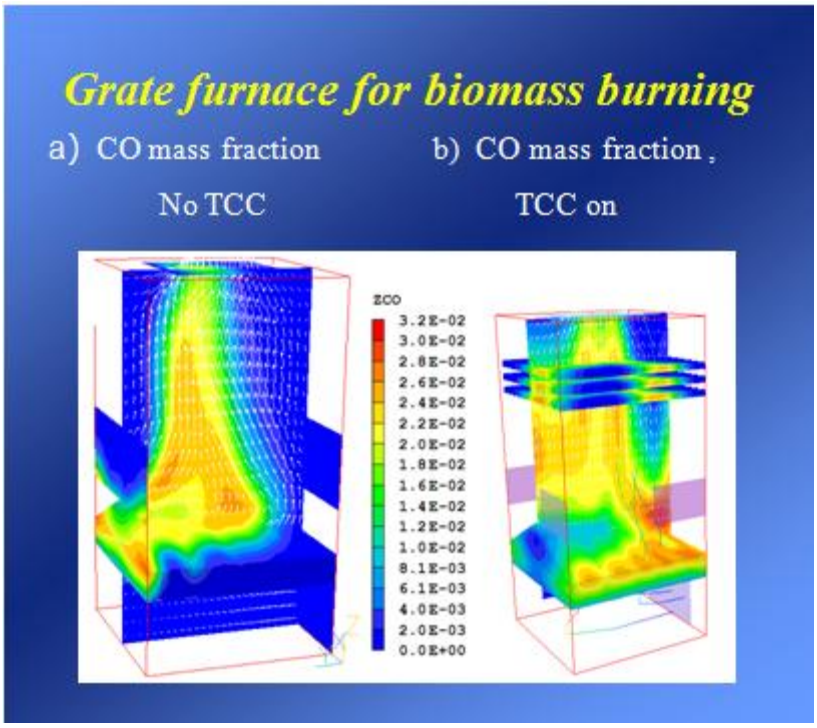
It dealt with *TCCs*, *Thermo-Chemical Cells*, of bayonet type for heat recovery. Mixture of one neutral gas (water steam) with combustible methane (CH_4) enters a smaller tube and after U-turn meets a layer of catalyst in annulus. Methane re-forming takes place and a mixture of two combustible gases ($CO+H_2$), called syngas, leaves the cell. External supply of heat is necessary for re-forming reactions to be completed. TCCs do not usually work solo, they are assembled in packets, bundles, or stacks of many tens if not of a few hundreds.

Modeling of single TCC presents no difficulties. It is their assemblies that give the simulation task a very challenging nature. The problem is that it is impractical if not impossible to make grid fine enough to capture details of flow and heat- mass transfer in the shell side along with the flow and heat fluxes over and inside all tubes and through their walls.



The way around this problem was found by employing space-averaged transport equations in the regions occupied by the stacks of thermo-chemical cells[1,2]. The procedure is called DRA, Distributed Resistance Analogy. It was successfully used earlier by author and his colleagues for modeling of shell- and tube heat exchangers, blast furnaces [3], stacks of fuel cells [4] and electrolyses batteries [5]. This technique has been significantly extended to accommodate the specifics of TCC. In fact, five interlinked sub-spaces are found necessary to be distributed in each TCC occupied region to represent the transfer of heat adequately.

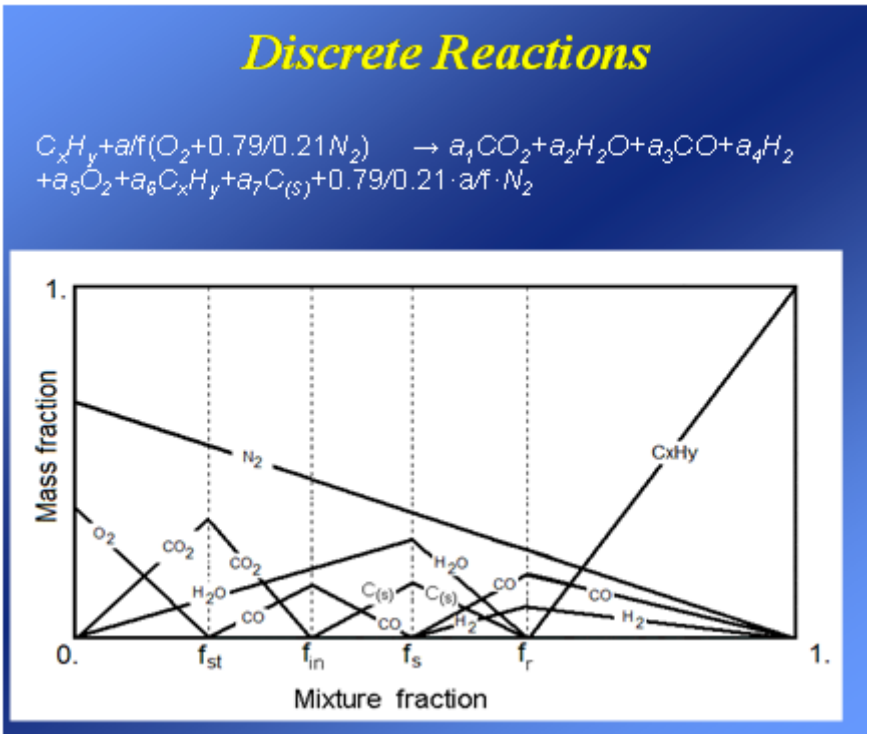
As a result, significant computational economy has been achieved by sub-spaces discretisation done in 1D manner over shell-side grid. When used with caution no much loses are expected in terms of predictive accuracy either. No more excessively fine grids to cover intricacies of TCCs inserts.



This screen shows two pictures of one particular case study illustrating the typical modeling results obtained by DRA methodology. The case in question is a grate furnace for biomass burning [6]. The wooden splinters are ignited on the grid through which the air is blowing, thus initiating combustion. Shown on the left picture are the contours of gas mixture temperature and velocity vectors.

As seen undisturbed plume of hot combustion products (mainly in red) is going up towards chimney. As clearly evident from the picture on the right the presence of thermo-chemical stack changes otherwise plume-like shape of CO mass fraction distribution. The heat taken out from the flow of combustion product is consumed by reforming reaction inside the cell tubes.

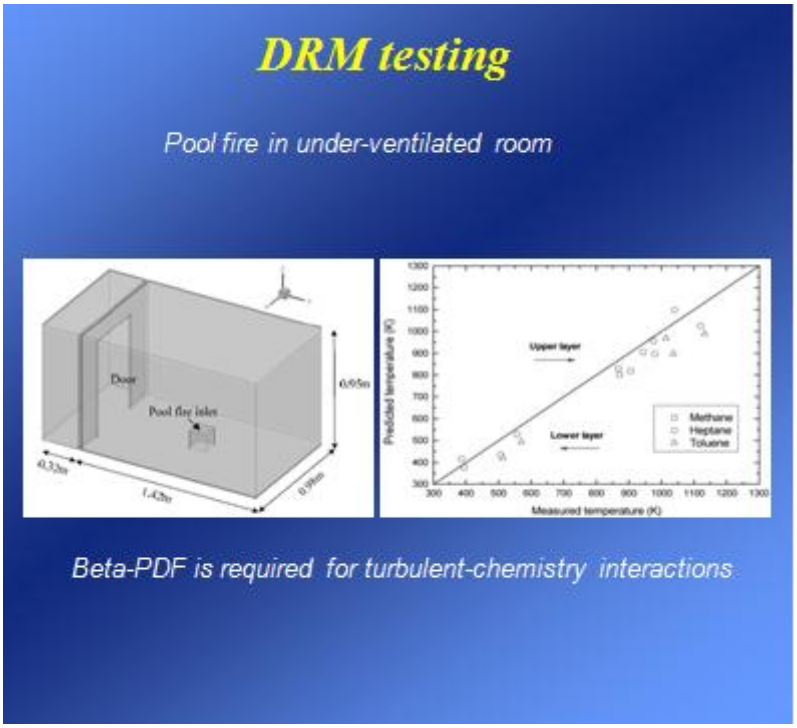
Because of temperature non-uniformities the distribution of CO along the tubes of TCC is also non-uniform. Changes of geometrical design and tuning of operating conditions are obviously desirable to provide more stable and balanced generation of syngas and consequently more efficient heat recovery. The transfer of heat to the in-tube streams of reforming mixture depends on thermo-physical properties of the combustion products which in turn, in not a minor part, are the functions of their composition.



The assumption that gas mixture composition is as for complete combustion products may lead to unnecessary loss of computational accuracy. To avoid this a model of appropriate trade-off between complexity, computational economy and predictive resolution is required to compute the product composition under different combustion scenarios in the shell-side flow across TCC stacks.

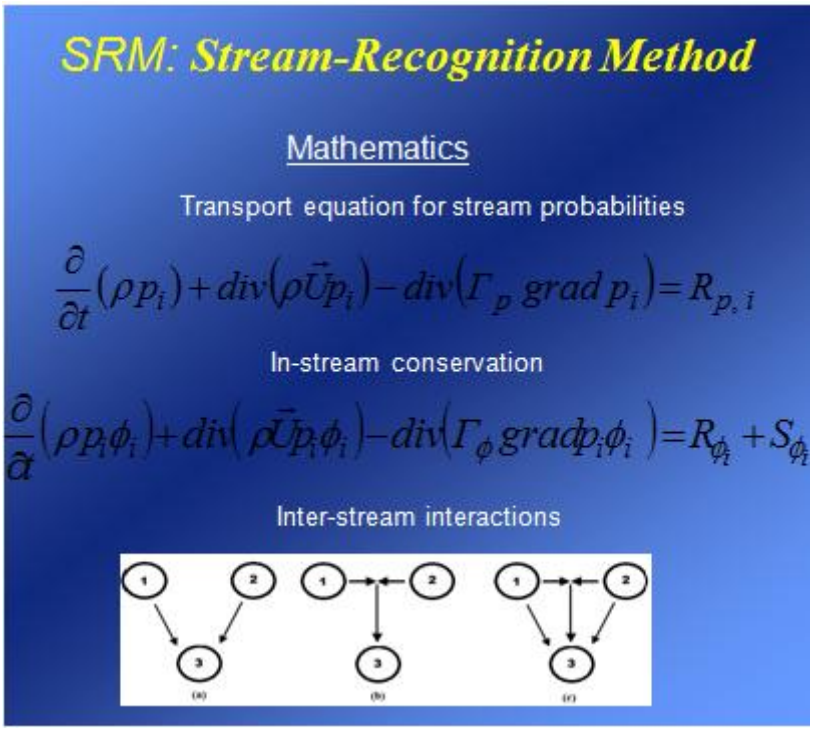
The current presenter recommends DRM, Discrete Reaction Model, which is described in details in [7-9] and in documents cited therein. Its easy to use and computationally economical algebraic nature could make it a model of choice for computer-power-hungry industrial CFD simulations. In the core of DRM approach lies the assumption of the existence of generic chemical equation of hydrocarbon oxidation. It is shown on the screen. Complete reaction product aside this equation postulates the presence of incomplete reaction products, such as carbon monoxide, molecular hydrogen and soot as solid carbon.

The problem with generic equation is that the number of unknown molecular coefficients at RHS is larger than number of atoms participating in reaction. Hence the closure problem. To circumvent this the discretization of generic reaction over O-atom or mixture fraction space guided by flame limit compositions is employed. The resulting diagram is presented on the screen. All the piecewise linear stretches are exact so that the closure problem avoided. The computational procedure uses conditional linear relationships on cell-by-cell basis to get product component mass fraction for computed fields of O-atom or mixture fractions.

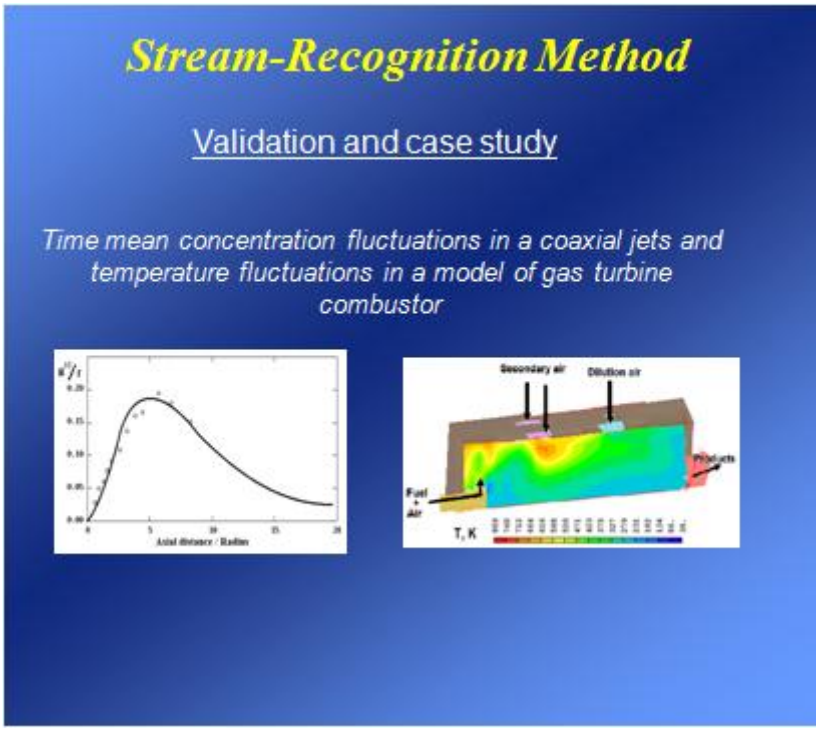


Comparisons with experiment shows fair agreement with developed theory. It is especially true for hydrocarbons with high soot propensity. One example of the comparison taken from [10] is shown on the screen for the temperatures inside under-ventilated room. In most of the cases considered so far the agreement seems to be reasonable for engineering purposes.

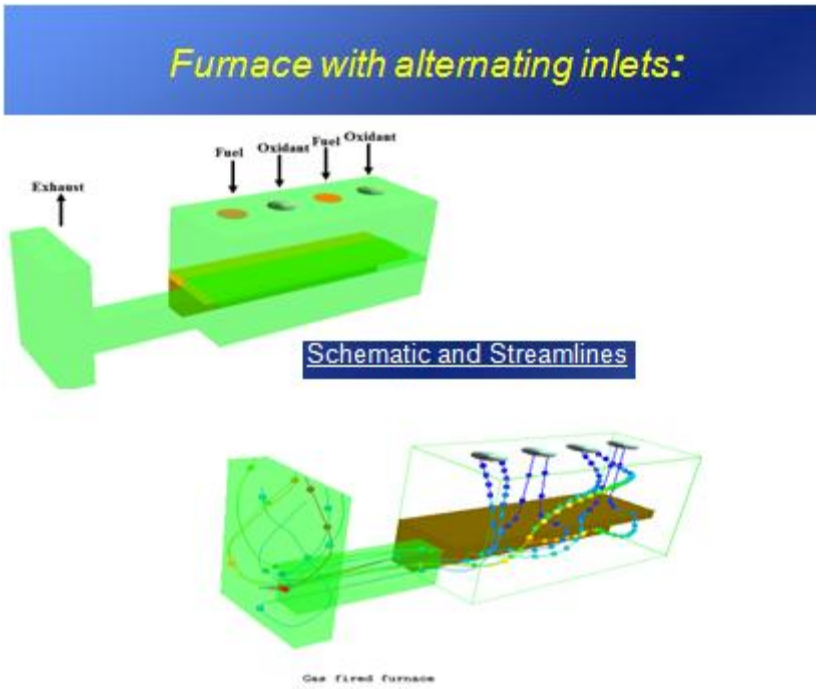
There is a trick, though. The beta-PDF, probability density function, was used to get model extension for probabilistic nature of turbulence-chemistry interaction. While beta-PDF construct is currently sort of industry-standard method, it requires an additional conservation equations for mixture fraction variance to be solved. In general the success of such an approach is intermittent to say the least. If something better could be developed which calculates the probabilistic properties rather than presumes them, the former should be given preferential consideration. This bring us to third model available, namely, a Stream Recognition Model of transported probabilities.



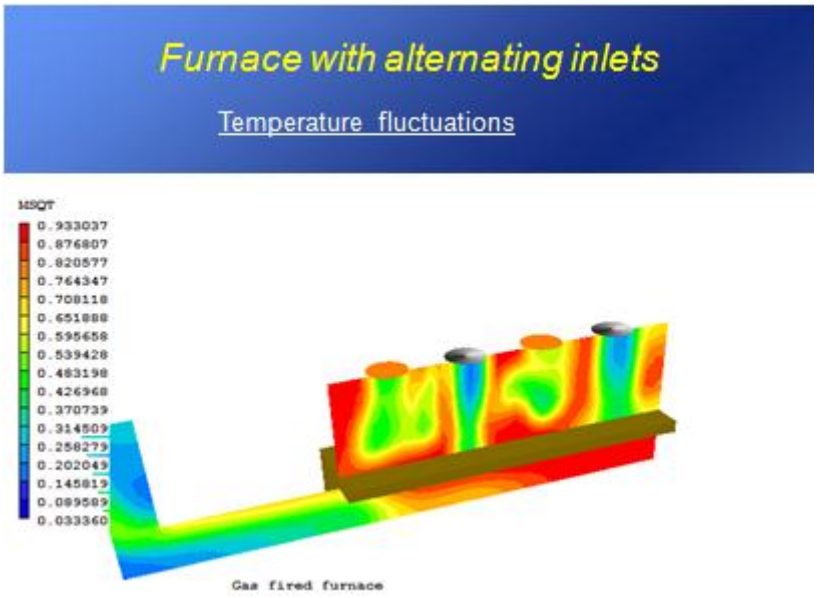
In SRM the three probabilities of two reactants and one product streams are assumed to be governed by conservation equations of general format [11]. Once calculated with unity conditions at appropriate inlets they are then used to compute source terms for in-stream conservation of physico-chemical flow properties. SRM uses three options for inter-stream interactions of probability fluxes, namely, direct injection, collision-driven and combination of both . Currently, with existing validation experience it is the latter option which is recommended for general use [12].



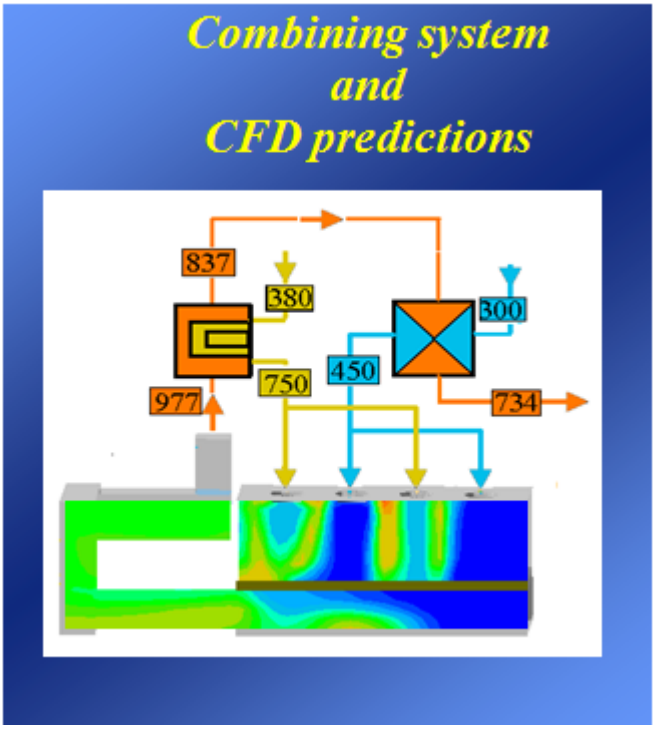
Shown on the screen are selected results of two case studies cited in [11]. One on the left was aimed at SRM validation. It shows that agreement with experiment is good. The picture on the right gives an impression of what sort of information should be expected from SRM simulations of the flow and chemical reactions in a model of gas turbine combustor. Distributions of temperature fluctuations exhibit expected locations of max and min areas.



The next case study is about industrial furnace with alternating inlets of reactants [13]. The two animated pictures show complex nature of 3D flow distributions inside the furnace operating space. On their way to the exhaust strong flow recirculation over the structure of working table is developed.

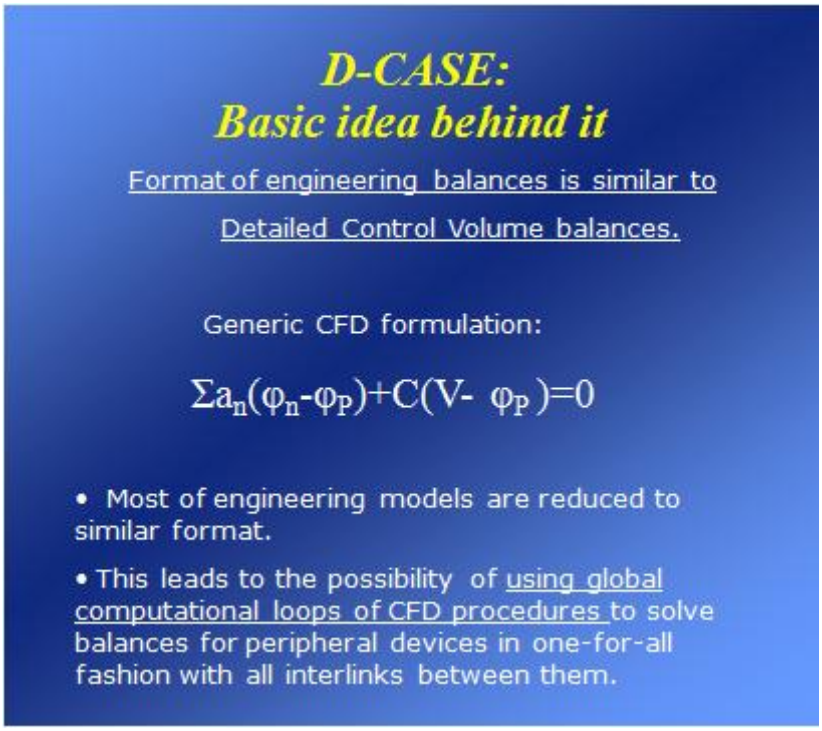


To generate results of RMS of temperature fluctuations shown on this screen SRM has been applied to the simulation of transition of combustion from the regime with low excess of air to the operating conditions of higher excess. The prediction shows expected trends and demonstrate the performance of SRM in transient and unsteady operation scenarios.



Most of the furnace operations are performed in thermo-technological loops/system where furnaces are surrounded with auxiliary and/or service devices such as heat exchangers [14]. As a rule the latter are fully coupled with each other and with, or through, a furnace. A screen snapshot shows one such system with two heat exchangers providing heat recovery.

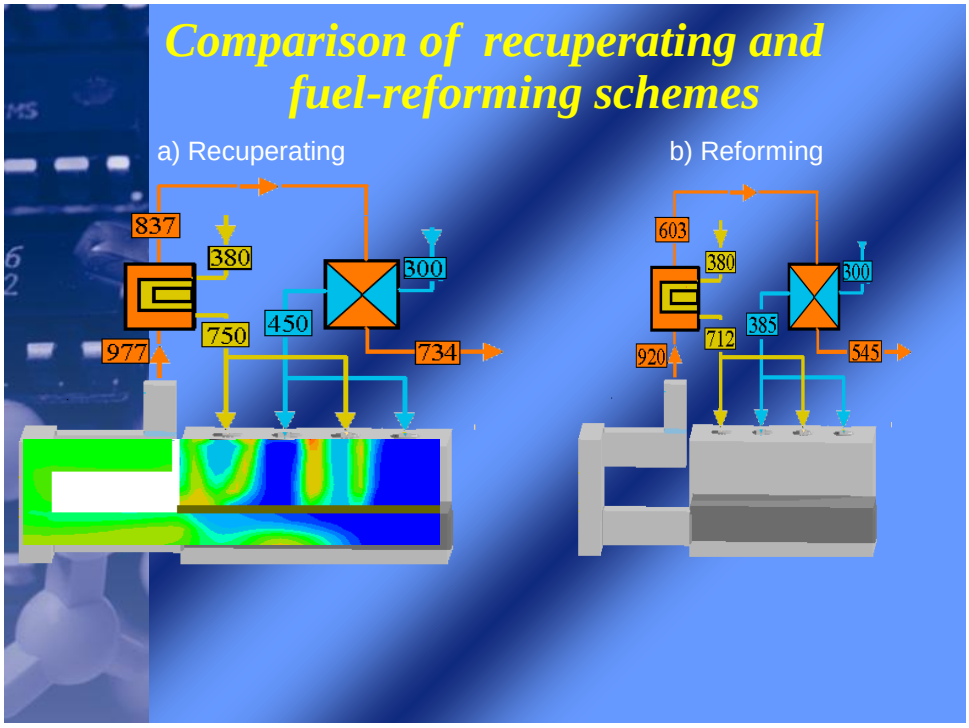
As seen all the processes taking place in any system organized in this way are closely connected: the conditions at the outlet of each device are input parameters for another one linked to it. CFD solvers should be made capable of obtaining simulations combining detailed numerical predictions with system evaluation.



D-CASE , Detail-Computational Analysis and System Evaluation, methodology has been invented to answer this need. It uses similarity between control-volume based cell balances of detailed CFD and overall balances and approximations of engineering type.

The fact is that most of engineering models are easily reduced to the format of CFD cell balances. This leads to the possibility of using global computational loops of CFD procedures to solve balances for peripheral devices in one-for-all fashion with all interlinks between them.

All what is needed is to select convenient cell and supply it with appropriate balance tunings, and computational links to its neighbor as system structure dictates.

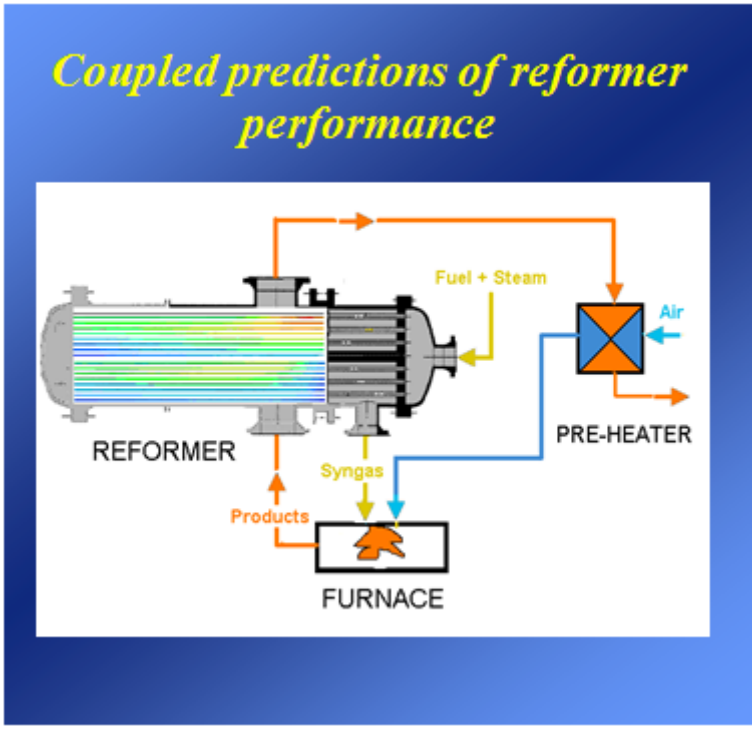


This screen snapshot and the next one display two examples of using D-CASE [15,16]. The one on current screen compares performances of two heat recovery systems computed with detailed furnace simulation.

For the scheme on the left, methane-steam conversion is not included, and the thermo-chemical reactor (yellow-orange rectangular) was presented as a cross-flow heat exchanger with a bayonet type bundle of tubes for recuperative heating of fuel gas entering the furnace. A recuperative cross-flow heat exchanger (cross in blue-red) is also considered to heat up the air entering the furnace.

A distinctive feature of the scheme on the right is the presence of a thermo-chemical reactor in which heating fuel is synthesized from a mixture of methane and water steam. The heat required for reaction is taken from gases emitted from the furnace. Still hot gases are then sent to the air heater. Heated air goes into furnace to maintain combustion.

Comparative analysis shows that thermo-chemical fuel regeneration significantly increases heat recovery mainly due to endothermic re-forming of initial mixture. Not only does the temperature of hot gases significantly decrease at the exit from TCR, the temperature of the converted syngas becomes noticeably lower than in the absence of conversion. The degree of heating of the furnace air entering the furnace is also reduced.

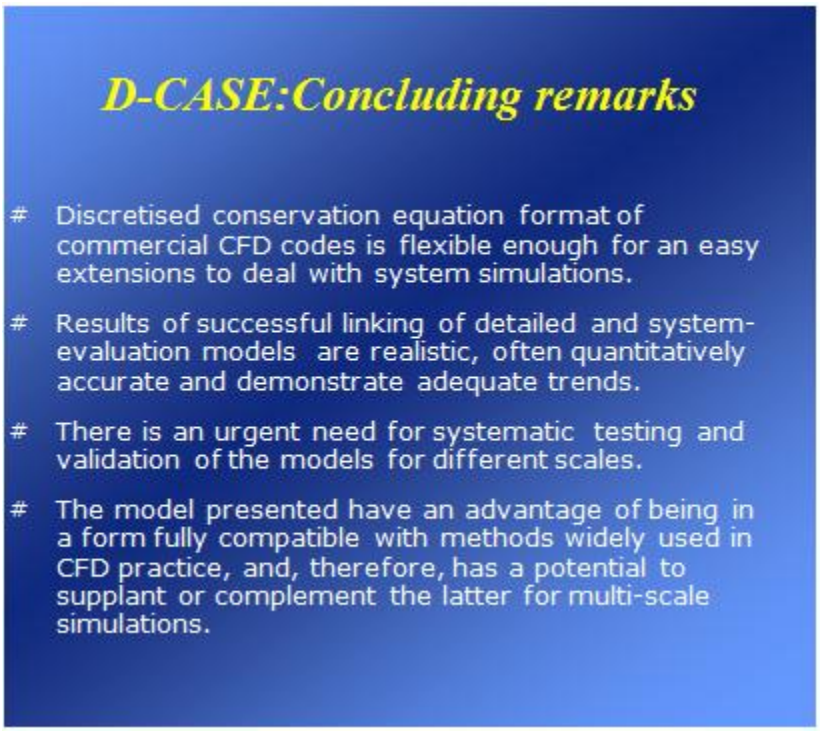


Using D-CASE there is no difficulty in switching detailed attention from one device to another.

Shown on the screen are detailed distributions of hydrogen mass fractions along the cells of thermo-chemical steam-reforming reactor. Note that for further computational economy the furnace has been represented as well-stirred reactor. The latter level of modeling is not a restriction of current method; the furnace could also be considered in 3D with additional computational cost.

As can be seen from picture on the screen, for system-controlled entry conditions, detailed calculations provide information on the distributions of the composition of the furnace gases over the entire volume of the reformer working space. This, in turn, provides an opportunity to more accurately determine structural and operational changes that, say, contribute to increasing degree of reactions completion.

Recent example of another successful D-CASE application to the technological system of ammonia cracking unit is reported in [17].



A few concluding remarks about D-CASE technique are displayed on the current screen. The most important of which are two of the followings:

- Discretised conservation equation format of commercial CFD codes is flexible enough for an easy extensions to deal with CFD/system simulations within a single computational loop.

- An implementational advantage; for D-CASE has an attached benefit of being in a form fully compatible with methods widely used in CFD practice, and, therefore, has a potential to complement the latter in CFD-in-system simulations.

As a general conclusion, it may be asserted with enough confidence that the all four computational models selected for assessment of their usefulness in coming projects and described in this presentation should be considered as useful predictive tools for research and engineering practice. They must be used with caution, though, but this is the case for any predictive approach.

In author's opinion, of all the furnace related models, the two , namely, the one for performance predictions of thermo-chemical heat recovery stacks, and also the methodology for detailed-computation analysis combined with system evaluation, could be prioritized as leading predictive devices for future tasks.

THANK YOU FOR YOUR ATTENTION

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