PROCESS SIMULATION OF FUEL CELL SYSTEMS: Recasting Detailed Models into System Models

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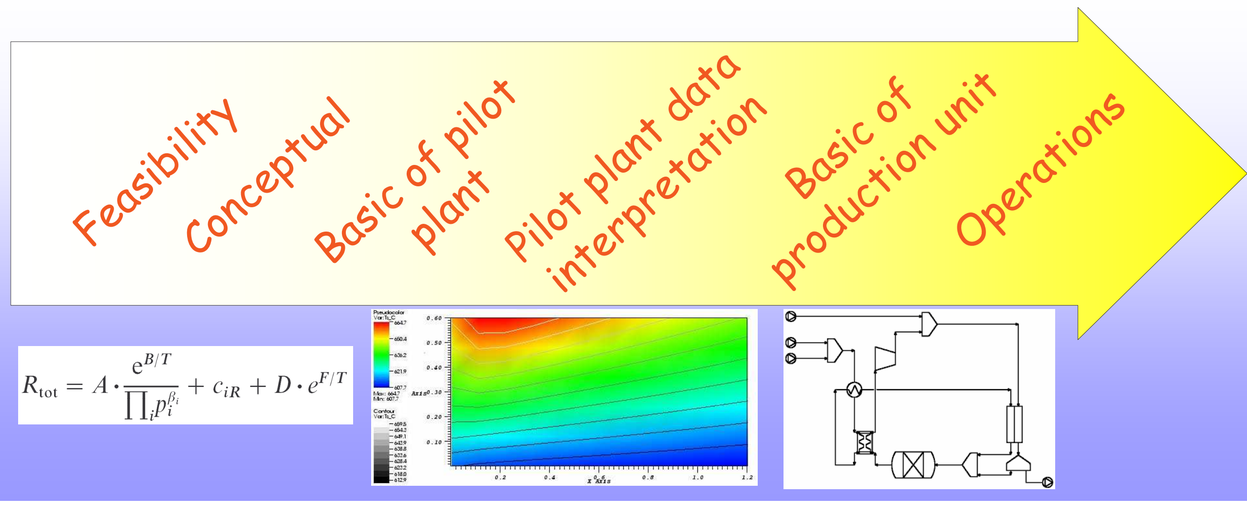
INTRODUCTION

The scope and requirements on fuel cell first-principle simulation models change throughout the different phases of product development.
On the **detailed** model MCFC D3S©, see our poster "*PROCESS SIMULATION OF FUEL CELL SYSTEMS: Identification Problems in Detailed Models*" B. Bosio, E. Arato, P. Greppi, P. Costa.
For system simulation a **simplified** model of each unit is desirable. Good practice dictates that between simplified and detailed model the **theoretical basis** should remain the same and the results should be **consistent**.



$$R_{\text{tot}} = A \cdot \frac{e^{B/T}}{\prod_i p_i^{\beta_i}} + c_{iR} + D \cdot e^{F/T}$$

LIBPF

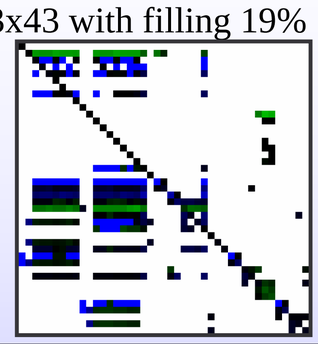
LIBPF (**LIB**rary for **P**rocess **F**lowsheeting) is the latest development of the group for fuel cell system modelling.
It is an object-oriented **C++** library designed to manipulate objects which are familiar to the process engineer:
- Quantities with physical **units of measurement**
- **Streams** with sub-streams
- **Flowsheeting**, graph analysis, flowsheet-in-flowsheet
- **Chemical species** and fluid **properties**

Its capabilities include:
- Interacting with plant control systems and SCADA via **OPC**
- Interacting with users through a graphical **User Interface**
- Chemical **Equilibrium** and VL **flashes**
- **Steady-state** or **dynamic** simulation
- Solving flowsheets **sequentially** or **simultaneously**
- Solving **NLAE** and **DAE** sets
- Basic **unit operations** (mixer, reactive heat exchangers, absorption columns ...)

See: Paolo Greppi "*Flowsheeting in C++*" European Modelling And Simulation Symposium Barcelona, Spain - October 4-6, 2006

A new, flexible, concentrated parameters fuel cell model has been deveoped within LIBPF.

LIBPF can compute dense or **sparse analytical derivatives**.
Example: sparse Jacobian of fuel cell system, 43x43 with filling 19%



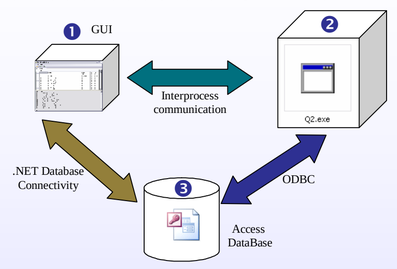
LIBPF enables personnel with little or **no skills in C++** to define the problem.

```
makeVertex<multihx> ("FC", "MCFC stack",
  oli("nReactions", 1)
     ("nMultiReactions", 1)
     ("nStreams", 2),
  ols("embeddedTypeReactions[00]", "reactionWGS_Eq")
     ("embeddedTypeMultiReactions[00]", "multiReaction_MCFC"));
makeEdge<streamV> ("ANIN", "Reformed cooled fuel", "REGHEX", "hotout", "FC", "anin");
makeEdge<streamV> ("ANOUT", "Anode outlet", "FC", "anout", "MIX2", "in1");
makeEdge<streamV> ("CATIN", "Cathode inlet", "MIX1", "out", "FC", "catin");
makeEdge<streamV> ("CATOUT", "Cathode outlet", "FC", "catout", "SPLIT", "in");
```

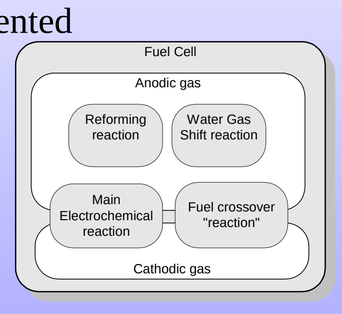
Specifying the problem is even easier.
No deep knowledge of C++ is required.

```
O("FC")->Q("netDuty")->set(0.0, "kW");  // heat losses
// anodic side
O("FC")->Q("deltaP", 0)->set(4.0, "mbar");
O("FC")->S("pressureOption", 0)->set("D");
O("FC")->I("reactionSides", 0)->I = 0;
// cathodic side
O("FC")->Q("deltaP", 1)->set(23.0, "mbar");
O("FC")->S("pressureOption", 1)->set("D");
// electrochemical reaction
O("FC:multiReactions[00]")->Q("H")->set(2.0*0.595, "m");
O("FC:multiReactions[00]")->Q("W")->set(1.195, "m");
O("FC:multiReactions[00]")->Q("Voffset")->set(-0.01663, "V");
O("FC:multiReactions[00]")->Q("z")->set(0.724412);
O("FC:multiReactions[00]")->Q("nCells")->set(300.0);
// heat transfer coefficients
O("FC")->Q("U", 0)->set(390.0, "W/(m2*K)");
O("FC")->Q("U", 1)->set(220.0, "W/(m2*K)");
```

LIBPF can make objects persistent to a relational database via **ODBC**



A multiple stream, multiple reaction, equilibrium- or fixed conversion **concentrated parameters fuel cell** model has been implemented



Visit http://www.libpf.com
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LIBPF

MATCHING

The fuel cell concentrated parameter model in LIBPF exhibits the same limitations common to all simplified models, i.e.:
- the values of the fields of distributed variables are not available,
- it is not predictive,
- the results will differ from those obtained with the distributed parameter model.

There is no way to cure the first two limitations; in particular the authors already highlighted in a previous work ("*Clean energy from sugarcane waste: feasibility study of an innovative application of bagasse and barbojo*" D. Dellepiane, B. Bosio, E. Arato Journal of Power Sources 122 (2003) 47–56) the importance of using detailed models also in system simulations to check that the operating point is compatible with local limits: the simulation results obtained were more substantial than the ones obtained from a system simulation where a simplified MCFC stack model was used.
For some applications of system modeling though it might be worth curing at least the last limitation, by matching the results of the detailed (distributed parameters) model and of the simplified (concentrated parameters) model, for a nominal operating point or for a range around it.
The matching is obtained by defining a suitable averaging scheme to represent the distributed fields as concentrated parameters, and by adding offsets to certain variables in the concentrated parameter. Results from the distributed parameters model can be used to define offset maps (as a of a selection of the inputs and operating specifications) or empirical correlations thereof.

CONCLUSIONS

The **MCFC D3S©** detailed model described elsewhere is an effective and validated standalone tool for fuel cell modeling, and can be used for system modeling within commercial process simulator software. To overcome the limitations of this approach to system modeling a concentrated parameter model was developed within **LIBPF**, the C++ library for process flowsheeting.
To reproduce accurately the results from the detailed model with the simplified model offsets or offset maps are included.
The use of these offsets allows to get accurate results in a certain range while retaining the fast resolution times characteristic of the concentrated parameter model. The price to pay is the inclusion of a black-box non-predictive "core" inside the first-principle concentrated parameters model.