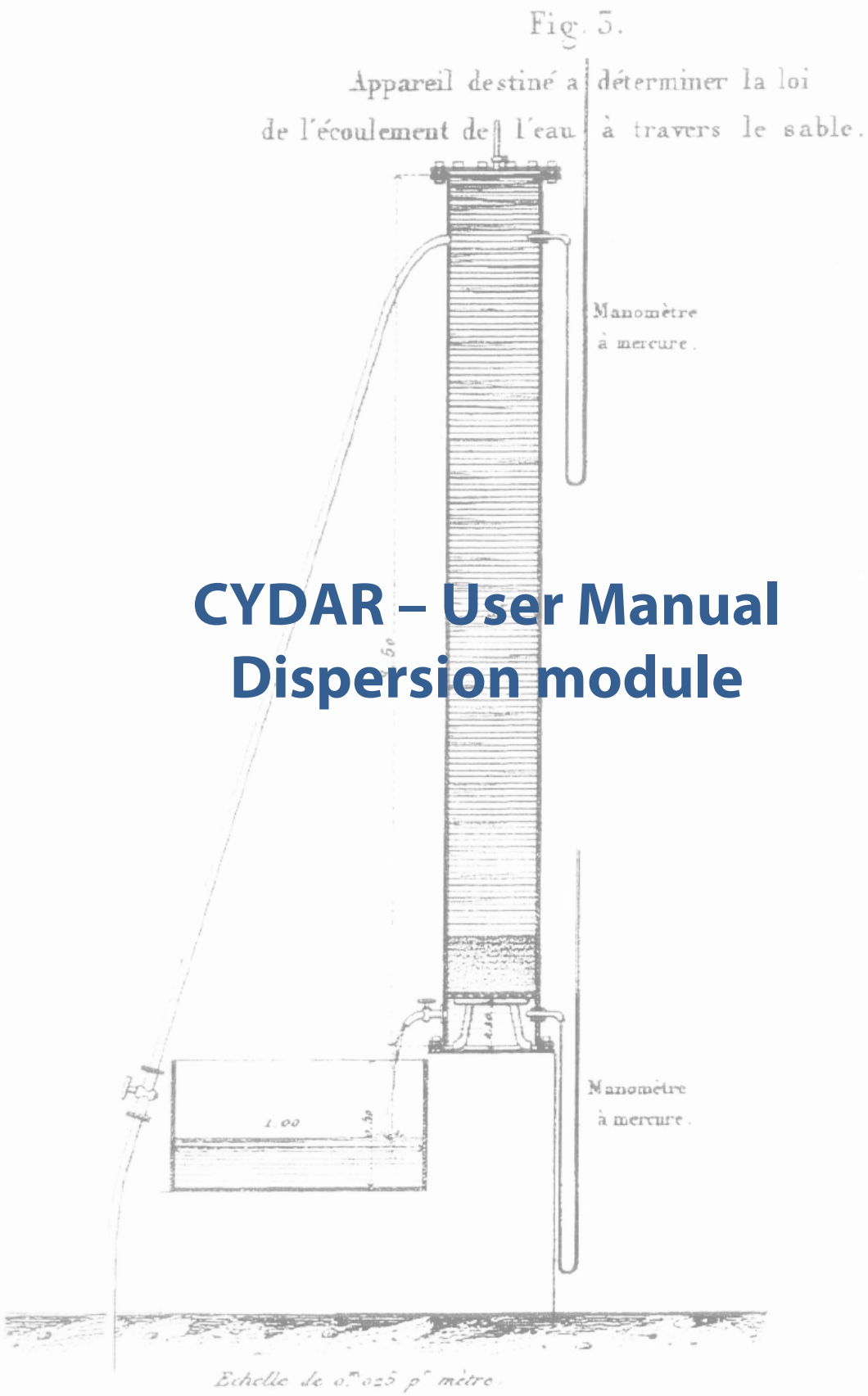
# CYDAR – User Manual
# Dispersion module



# CYDAR – USER MANUAL
# Dispersion module

# Dispersion module

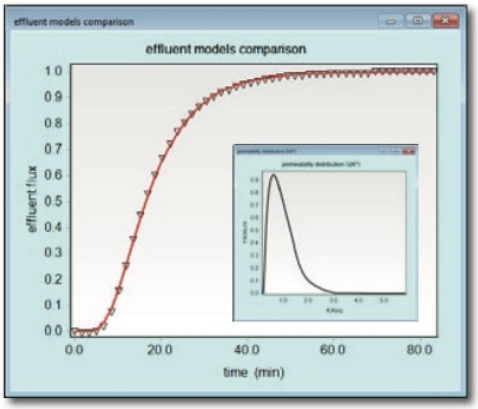
This notice describes the functionalities of the dispersion module of CYDAR. The functionalities of CYDAR common for all modules are described in a separate document ("CYDAR Common Features User Manual").

All User Manuals are available on our website www.cydarex.fr.

## CYDAR – Overview of the Dispersion Module

In CYDAR 2017, we are introducing a new dispersion / tracer module. Dispersion experiments give indication on the homogeneity of the sample, by analyzing dispersion of an injected solution at concentration $C_{in}$ with a solution at concentration $C_0$ present in sample.

- 4 models have been implemented: Classical, Koval, Coats and Smith, and Stratified.
- Temperature corrections and normalization are available…




**Example of dispersion experiments interpreted using the standard dispersion model (in red) and the stratified model (insert) described in paper SCA2015-014.**

# Launching the Dispersion Module

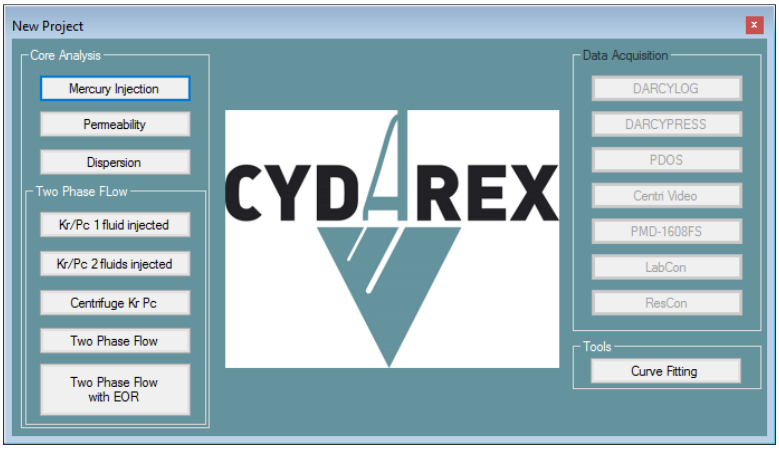



*Figure 1: CYDAR new project window.*

The Dispersion Module is launch from the New Project window, by selecting "Dispersion." If you are running the Dispersion module in Demo mode, you might be prompt to enter an activation passcode. Contact Cydarex to obtain this code.

# Dispersion main window

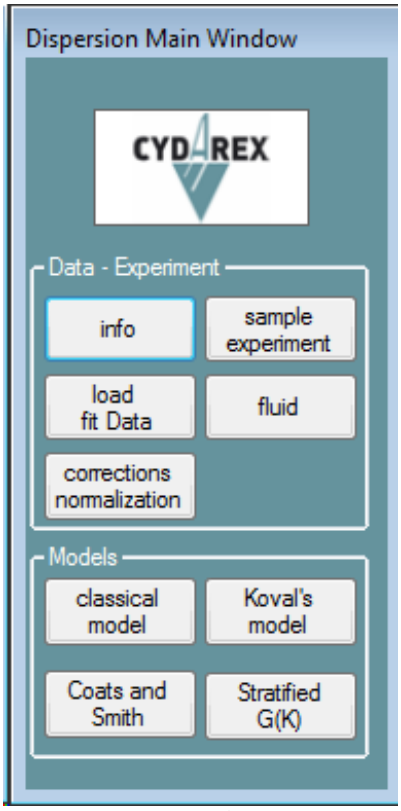



*Figure 2: Main window of dispersion module.*

**Data - Experiment frame:**

"**Info**": common to all modules, allows entering information regarding the sample and experience. None of this information is used for calculation.
"**sample/experiment**": dimensions and porosity of a cylindrical sample, injection, effluent and profiles data type (concentration or flux), Reynolds and Peclet numbers.
"**load/fit data**": input data spreadsheet, data corrections, possibility to edit and fit data.
"**Fluid**": fluid properties window, used only for the Reynolds calculation.
"**corrections/normalization**": temperature correction and normalization of the data, time correction for the profiles.

**Models frame:**

"**Classical model**": fit with the "classical" dispersion model.
"**Koval's model**": fit with the Koval's model.
"**Coats and Smith**": Simulation and optimization using the Coats and Smith model.
"**Stratified G(K)**": interpretation of the experiment with a stratified medium giving a distribution of permeability.

# Sample and experiment properties

## Sample frame

The sample is assumed to be cylindrical. The length and either the diameter, the section, or the pore volume if the porosity is known need to be entered (Figure 3). The permeability is optional and is only used to calculate the Reynolds and Peclet numbers displayed in the experiment frame.

## Experiment frame

First the user chooses if the injected concentration is greater than the initial concentration in place $C_{in} > C_0$ or the opposite situation $C_0 > C_{in}$. The flow rate is needed for calculation. The diffusion coefficient is optional and used only for calculation of the Péclet number.

The Péclet number represents the ratio of advective transport over diffusive transport, and is defined as follow:

$$Pe = \frac{V\sqrt{K}}{D_m},$$

where V is the front velocity $V = Q/(A\Phi)$, with A the sample section, Q the flow rate, and $\phi$ the porosity. K is the permeability and $D_m$ is the coefficient of molecular diffusion, with a default value of 2. $10^{-5}$ $cm^2/s$.

The Reynolds number is the ratio of inertial forces to viscous forces, and is defined as follow:

$$Re = \frac{\rho Q\sqrt{K}}{A\,\Phi\mu},$$

where $\rho$ and μ are the density and viscosity of the fluid.

Finally, the user selects what are the effluent and profiles data type: flux or concentration. Practically the flux is measured at the outlet, and the profiles are concentrations.

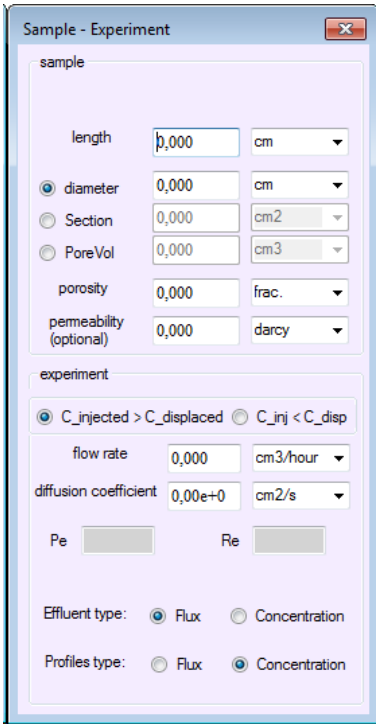



*Figure 3: Sample window*

# Data processing

As in other modules (see CYDAR User Manual Common Features), there are two main groups of data:

- Raw data are the direct experimental data that have been uploaded.
- Corrected and normalized data are the data used for interpretation. These data can have been corrected or normalized, and have been fitted.

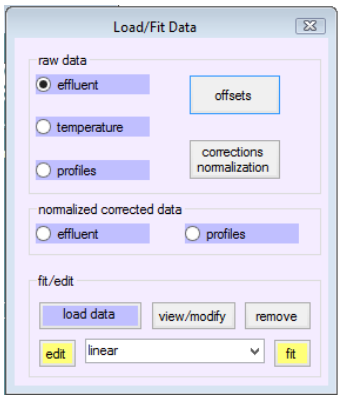



*Figure 4: Load/Fit Data window, allows performing data offset correction, editing, etc…*

The "Load/Fit window" (Figure 4) is used to:

- Load data.
- Open the "Data offset corrections" window (Figure 5).
- Open the "temperature correction and normalization" window (Figure 6).
- Edit and perform fit. A fit needs to be performed for each data set. A linear fit is the default fit, and the "fit" button needs to be pressed.

## Data units

All interpretations are performed on data that are assumed to be normalized. Therefore, units of the measurements have no impact on the interpretation. For instance, the effluent can be a tension or a density measure, the profiles can be X ray scan or resistivity measurement; in all cases the normalization will lead to dimensionless physical quantities:

$$Y^* = \frac{Y_{exp} - Y_{min}}{Y_{max} - Y_{min}}$$

$Y^*$ is the normalized dimensionless physical quantity. $Y_{exp}$ is the measurements of this physical quantity (tension, density, X ray, etc.). $Y_{max}$ and $Y_{min}$ are the extrema with the same unit than $Y_{exp}$ used for normalization. See below to know how to perform normalization and correction.

The other physical values, like temperature, time, and distance, have the proper unit type.

## Raw data

There are three different data sets:

- Effluent: measurements versus time.
- Temperature: temperature versus time.
- Profiles: a set of measurements at different locations along the sample performed at different time.

The effluent and profiles raw data cannot be edited, but they are used to calculate corrected and normalized data. These data can be edited. In CYDAR, profile data cannot be edited.

In CYDAR, the corrected data are the data used for calculation and interpretation; see the recommended way to process data below.

The temperature data is used for measurements correction (see below). The calculation uses the analytical fit of the data. Therefore, any edition and fit must be done before calculation of the correction.

Offset correction, due to dead volume for example, can be perform from the "Data offset corrections" window (Figure 5). This window is open with the button "offsets" on window "Load/Fit window" (Figure 4).

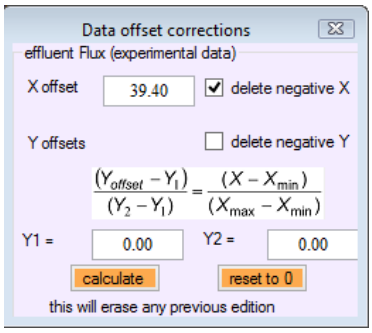



*Figure 5: Data offset correction window.*

## Corrected and normalized data

Data are calculated from the effluent and profiles raw data. Figure 6 shows the dedicated window with the different entries.

### *Temperature correction and normalization*

The temperature correction and normalization are performed on both effluent and profiles data. The different parameters units are assumed to be similar to the data's units. All parameters must be set before calculation by pressing the "calculation" button.

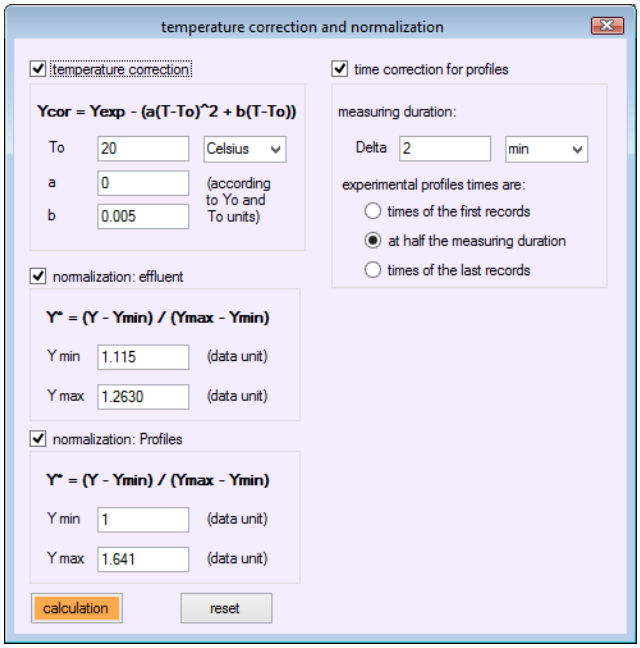



*Figure 6: Temperature correction, normalization and time correction for profiles window.*

The effect of the temperature correction can be checked on the graph with the raw data. These graphs can be opened in the "Graphs" window: "effluent" and "profiles" in frame "experimental data" (Figure 16).

The Figure 7 shows an example of the effluent graph displaying the raw data (in black), the correction by temperature before normalization (in green) and the minimum and maximum value used for normalization (horizontal lines). Any change in the parameters will update graphs.

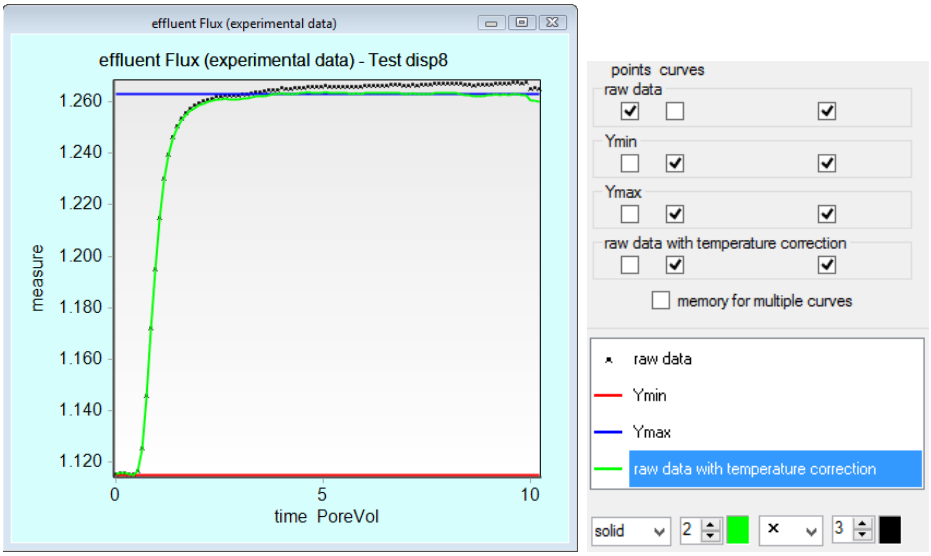



*Figure 7: a graph with an example of the temperature correction effect and the normalization extrema displayed. The raw data is in black, the green curve is the corrected data; the blue and red horizontal lines are $Y_{min}$ and $Y_{max}$.*

When the correction and normalization are done, the calculated data can be displayed on the graphs of the"Models (Fit)" section of the "Graph" window (Figure 16). All the graphs in this section display these calculated data as "corrected and normalized data". After correction, a fit needs to be run.

The temperature correction is given by:

$$Y_{cor} = Y_{exp} - b(T - T_0) - a(T - T_0)^2$$

$Y_{cor}$ is the corrected measurement before normalization. $Y_{exp}$ is the raw data. $T_0$ is the reference temperature. And a and b are coefficients with proper units.

The normalization is simply:

$$Y^* = \frac{Y_{cor} - Y_{min}}{Y_{max} - Y_{min}}$$

***Profile time correction***

A profile is a set of measurements along the sample started at a given time. Depending on the setup, these measurements cannot be simultaneous but sequential. In other words, the profile is not an instantaneous photography of the experiment. It can be useful to account for the duration of the measurements.

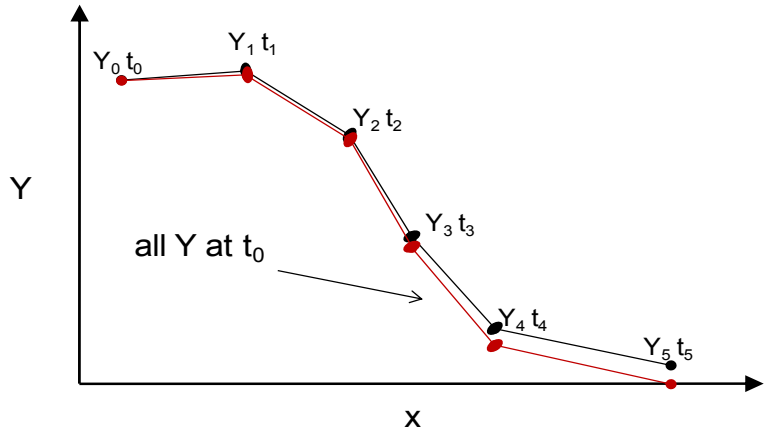



*Figure 8: sketch of the measuring duration effect on a profile measurement.*

Figure 8 shows the effect on the profiles measurements when the duration of measurements is not negligible. In this hypothetic experiment, one profile measurement was started at $t_0$. The points were taken

sequentially at different increasing time: $t_1$ to $t_5$. The red line would be the profile obtained with simultaneous measurements.

The dispersion module offers the possibility to account for such effect. In practice, the corrected and normalized experimental data are not modified in CYDAR. But the models, simulations ,and calculations account for the correction. For instance, when a fit is performed with a model the optimization of the parameters is done on corrected profiles. And, the fit curves are displayed with the same time than the experimental one.

The user enters the average measuring duration in the "temperature correction and normalization" window (Figure 6). The user chooses also what the times for profiles loaded in the spreadsheet are. "Experimental profiles times are":

- "times of the first records";
- at half of the measuring duration;
- "times of the last records".

# Injection and boundary conditions

Very often experiments with a continuous injection with a constant concentration $C_{in}$ are interpreted using analytical solution obtained assuming constant concentration at the inlet. However, the physical boundary condition is a constant density flux. Experiments on micromodels have shown that concentration at the inlet of the porous medium is not constant. Practically we inject a fluid at a constant concentration but this is the flux density that is constant, see for instance the 2015 SCA paper from Lenormand et al. (Lenormand, Lenormand, & Bauget, 2015).

Therefore, the interpretation in CYDAR assumes a continuous injection of a constant flux from time t=0:

$$F_{in}(t) = QAC_{in}u(t) \text{ with } u=\begin{cases} 0 & t < 0 \\ \frac{1}{2} & t = 0 \\ 1 & t > 0 \end{cases}$$

$F_{in}(t)$ is the flux density which is zero before the start of the injection then constant during the experiment. $C_{in}$ is the concentration of the injected fluid. Q is the volume flow rate that is constant as well. And A is the sample section. $C_{in}$ may either be smaller or greater that the initial concentration $C_0$ in place. The entries to specify the injection properties are on the window "Sample – Experiment" (Figure 3), see below.

The outlet has no effect on the spreading in the sample. The analytical solutions are obtained assuming a zero concentration flux at the infinite. The outlet boundary condition used in the simulation for the Coats and Smith model is a zero second derivative of concentration according to space: $\partial^2 C/\partial x^2 = 0$.

# Hydrodynamic dispersion model

## *Analytical solutions*

The model corresponds to:

$$F = V\phi\left(C - \alpha\frac{\partial C}{\partial x}\right),$$

$$\frac{\partial C}{\partial t} + \frac{1}{\phi}\frac{\partial F}{\partial x} = 0,$$

with F the flux density, C the concentration, V the front velocity ($V = Q/(A\phi)$), $\alpha$ the dispersivity.

With the boundary conditions given above, a constant flux injection and a zero concentration at the infinite, the analytical solutions for the flux and concentration are:

$$f = \frac{f_{in}}{2}\left(\operatorname{erfc}(z_1) + \exp\left(\frac{x}{\alpha}\right)\operatorname{erfc}(z_2)\right),$$

$$C = \frac{C_{in}\,V}{2}\left(\operatorname{erfc}(z_1) - \left(1 + \frac{1}{\alpha}(x + Vt)\right)\exp\left(\frac{x}{\alpha}\right)\operatorname{erfc}(z_2) + 2\left(\frac{Vt}{\pi\alpha}\right)^{\frac{1}{2}}\exp(-{z_1}^2)\right),$$

with

$$z_1 = \frac{x - Vt}{2(\alpha Vt)^{1/2}},$$

and

$$z_2 = \frac{x + Vt}{2(\alpha Vt)^{1/2}}.$$

See for instance (Lenormand, Lenormand, & Bauget, 2015) or equation 13 of the Coats and Smith 1964 paper (Coats & Smith, 1964).

**Remark:** the concentration equation given in the SCA paper contains a typo: the factor V and 2 are missing.

### *Interpretation with the hydrodynamic dispersion model*

The dedicated window is open by clicking the button "model classic". Figure 9 shows this window.

In the frame "graphs" the user can open or close some graphs where the result of the fit can be displayed. The fit can be done on effluent and/or profiles data, the choice is done using the corresponding checkboxes. The user can also choose which profiles will be used for the fit calculation (group of checkboxes in the window bottom).

The fit is performed by optimizing the dispersivity. The textbox with a white background is the initial guess, and the one with a light grey background is the value corresponding to the best fit.

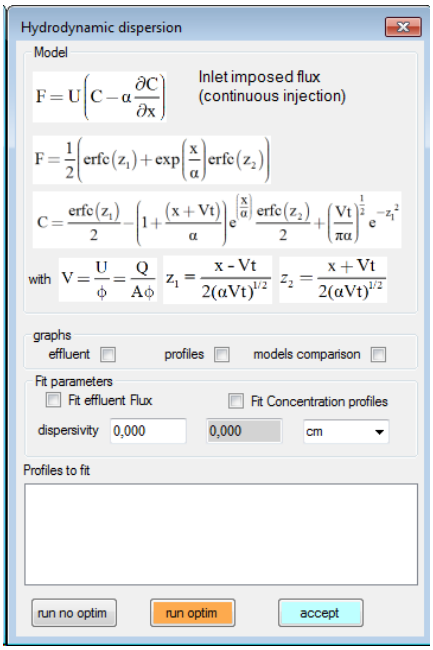



*Figure 9: the "Hydrodynamic dispersion" model window.*

The "run no optim" button allows to calculate the analytical solutions for the effluent and profiles using the initial guess without any optimization. The "run optim" launches the fit. The "accept" button passes the value of the best fit to the initial guess textbox and set this value as the current dispersivity.

**Remark:** only the value displayed in the initial guess textbox is saved in the project file.

# Koval's model

The Koval's model is a one dimensional homogenized model of viscous fingering in miscible flow. It not only accounts for viscosities ratio effect but also for the medium heterogeneities through a heterogeneous factor H, see details in the original paper of Koval (Koval, 1963).

In the dispersion module of Cydar, only the heterogeneity factor is considered. There is no viscosity ratio.

## Analytical solutions

The model is:

$$F = \frac{HC}{C(H-1)+1},$$

$$\frac{\partial C}{\partial t} + \frac{1}{\phi}\frac{\partial F}{\partial x} = 0.$$

The flux solution is:

$$f = \begin{cases} 0 & t \le \frac{x}{Vt} \\ \left(H - \frac{\sqrt{Hx/(Vt)}}{H-1}\right) & \\ 1 & t \ge \frac{xH}{V} \end{cases}$$

And the concentration solution is:

$$c = \begin{cases} 1 & x \le \frac{Vt}{H} \\ \left(\frac{\sqrt{HVt/x - 1}}{H-1}\right) & \\ 0 & x \ge HVt \end{cases}$$

## Interpretation with the Koval's model

Figure 10 shows the Cydar's window used for interpretation with Koval's model.

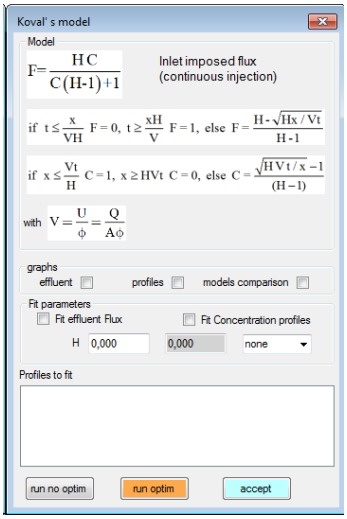



*Figure 10: the "Koval's model" window.*

Entries and principle are the same that with the hydrodynamic dispersion model. The only difference is that the optimized parameter is the heterogeneity factor.

# The Coats and Smith model

In porous media, dead volumes may exist and can lead to long time tail behavior. Coat and Smith have adapted the hydrodynamic model (see above) to this kind of behavior by adding a mass transfer equation between the flowing and the stagnant regions (Coats & Smith, 1964).

## The model

The flux-concentration relation is the same than in the hydrodynamic dispersion model:

$$F = V\phi\left(C - \alpha\frac{\partial C}{\partial x}\right).$$

In the mass balance equation a new term accounting for the non-flowing fraction of fluid is added:

$$(1 - S_f)\frac{\partial C_s}{\partial t} + S_f\frac{\partial C}{\partial t} + \frac{1}{\phi}\frac{\partial F}{\partial x} = 0,$$

$$(1 - S_f)\frac{\partial C_s}{\partial t} = K(C - C_s),$$

with $C_s$ the concentration in the non-flowing fraction of fluid, $S_f$ the fraction of flowing fluid and K the rate of transfer between flowing and stagnant volumes.

## Interpretation with the Coats and Smith model

Figure 11 shows the "Coats and Smith model" window. The optimization is done on the effluent data. Three parameters can be adjusted: the dispersivity, the transfer rate and the flowing fraction. The textboxes with the white background are the values used for simulation and the initial guesses of the optimization. The boxes with the light grey background are the final value of the optimization. The root mean square error is indicated. The user chooses which parameter to optimize using the checkboxes on the left.

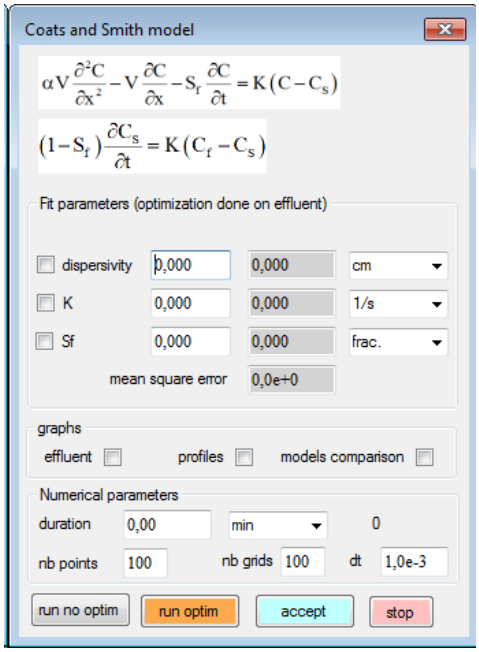



*Figure 11: the "Coats and Smith model" window.*

The numerical parameters are:

- the simulation duration;
- the number of outputs asked ("nb points"), asked because some points may be added to correspond to the times for profiles;
- the number of grids ("nb grids");
- the dimensionless time step "dt".

The buttons:

- "run no optim" starts one simulation using the values entered in the textboxes with white background;
- "run optim" launch the optimization on the selected parameters;
- "accept" passes the optimized values to the initial guesses;

- "stop" stops running simulation and optimization.

As for the other model, only the value displayed in the initial guess textbox is saved in the project file.

**Remark:** The simulation data are not saved, only the parameters displayed on the model window are saved. Therefore, to display the simulation outputs on graph, the simulation must be rerun after the opening of a project.

# Stratified model

## Model

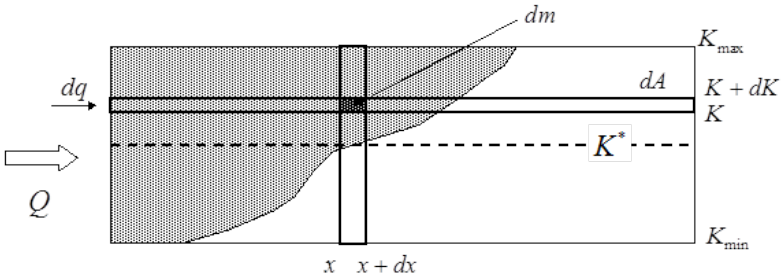



*Figure 12: Perfectly layered medium: principle of the calculation of tracer transport.*

Stratified media have been extensively used as model of heterogeneous media either for immiscible or miscible flow. The heterogeneous porous medium is represented by a perfectly layered medium with a permeability distribution function $G(K)$. Microscopic dispersion is assumed to be negligible and the tracer follows the streamlines. To simplify the calculation, the layers are re-arranged with increasing permeability (Figure 12). At a given time, the front of tracer is calculated using the flow rate in each layer and the concentration, by averaging over the cross-section:

$$C(x,t) = C_0 \int_{K^*}^{K_{max}} G(K)dK,$$

where $K^* = \frac{K_{eq}}{V}\frac{x}{t}$ is the lower limit of the invaded layers and $K_{eq}$ is the effective permeability. The flux at the same position is calculated by summing the flow rates in all invaded layers:

$$F(x,t) = \int_{K^*}^{K_{max}} C_0 \; dq = C_0 Q \frac{1}{K_{eq}} \int_{K^*}^{K_{max}} K \; G(K)dK.$$

The curve can be determined numerically by elimination of the parameter $K^*$.

The dispersion module of CYDAR allows the calculation of G(K/$K_{eq}$) from the profiles and the effluent data, and the calculation of the profiles from these permeability distributions.

## Interpretation with the stratified model

Figure 13 shows the "stratified model" window. The beta coefficient is a parameter allowing to account for non convective spreading.

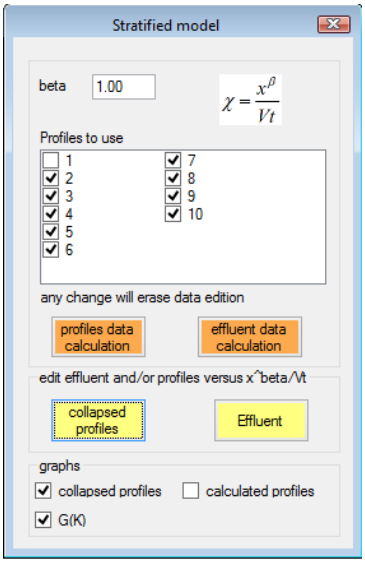



*Figure 13: "Stratified model" window.*

The orange buttons "profiles data calculation" and "effluent data calculation" launch the calculation of the collapsed profiles and the effluent versus $x^\beta/(Vt)$. The collapsed profiles are all the selected profiles grouped in one data that can be fit using splines for instance. Figure 14 shows an example of a graph displaying calculated collapsed profiles, its fit and the fit of the effluent data.

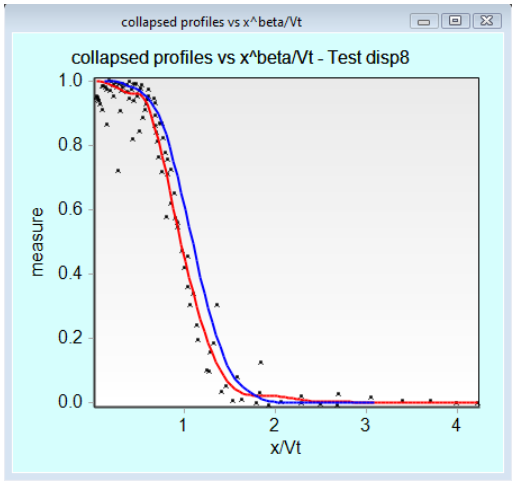



*Figure 14: "collapsed profiles" graph displaying an example of calculated collapsed profiles (black dots), its fit (red line) and the fit of the effluent data versus $x^\beta/(Vt)$ (blue line).*

The yellow buttons on the "stratified model" window open the "edit points panel" for the collapsed profiles and effluent data from which editing and fitting can be performed.

The two permeability distributions are calculated from the fits of the collapsed profiles and the effluent versus $x^\beta/(Vt)$.

Any new calculation erases previous data edition and existing fit.

The checkboxes in the "graphs" frame open the corresponding graphs:

- "collapsed profiles" opens the graph where collapsed profiles data, its fit and the fit of effluent data versus $x^\beta/(Vt)$ can be displayed;
- "G(K)" is the graph allowing to display the two permeability distributions versus $K/K_{eq}$ calculated from the collapsed profiles fit and the effluent fit (Figure 15);
- on "calculated profiles" the user can display the profiles calculated from these G(K).

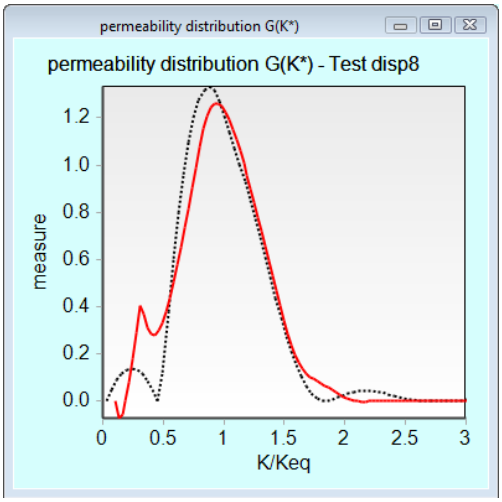



*Figure 15: example of permeability distributions calculated from profiles (dot line) and effluent (red line).*

# Graphs

As in other CYDAR modules, the menu "view" opens a window from which the different graphs can be open or closed (Figure 16).

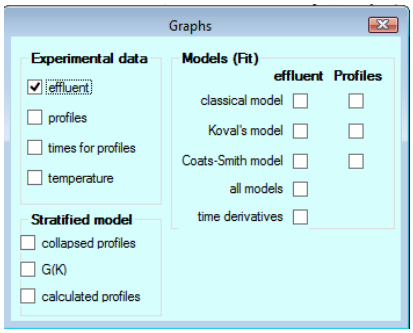



*Figure 16: "Graphs" window allowing to display the different graphs.*

Frame "Experimental data":

- "effluent": graph with the effluent data loaded and before any correction, the extrema used for normalization and the result of temperature correction before normalization;
- "profiles": idem with the profiles data;
- "times for profiles": the times loaded with the profiles;
- "temperature": the temperature data used for the temperature correction.

Frame "Models (Fit)":

- For each model: graphs with the normalized and corrected data for "effluent" and "profiles" and the output of the corresponding model;
- "all models": graph with the comparison of the three effluents calculated;
- "time derivative": graph with effluent time derivatives of the normalized data and the calculated data.

Frame "Stratified model":

- "collapsed profiles": graph with collapsed profiles data, its fit and the fit of effluent data versus $x^{\beta}/(Vt)$;
- "G(K)": graph with the two permeability distributions versus $K/K_{eq}$ calculated from the collapsed profiles fit and the effluent fit;

- "calculated profiles": graph with the profiles calculated from these G(K).

# Recommended data processing

1. Entering the general information
2. Entering the sample properties and experimental characteristic
3. Entering the fluid properties (used only for the Reynolds calculation)
4. Loading the raw data:
    a. no editing for the effluent and profiles
    b. editing the temperature if necessary because this is its analytical fit which will be used for correction
5. Performing the offsets correction, for instance that is the way to take into account the dead volume effect on the effluent measurement
6. Performing the normalization, the temperature correction and the time correction for the profiles if desired, giving the data used for interpretation
7. Performing interpretation with the different models

# Tutorials

Tutorials files can be downloaded from CYDAREX website. For the module Dispersion, the following files are available:

- Dispersion_Tutorial_SCA8.xlsx
- SCA_8_effluent.cydx
- SCA_8_profiles.cydx

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2. Koval, A. (1963, June). A Method for Predicting the Performance of Unstable Miscible Displacement in Heterogeneous Media. *SPE Journal* , 145-154.
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