Comsol Multiphysics in Education – Chemical Reactions, Heat and Mass Transfer

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Abstract: In our Master program entitled "Verfahrenstechnik / Process Engineering" the main focus is placed on the use of computational methods, including computer exercises. This paper will provide the plan of a particular course entitled "Transportprozesse" (Transport Processes or Transport Phenomena).

The contents of the lecture and exercises encompass mass and heat transfer, chemical reactions and fluid mechanics. That includes "single physic" and "multi physic", steady state and transient processes. The selected problems are solved analytically and numerically. The software called Comsol Multiphysics is used to find the numerical solution. The organization of the course, its aims, the priorities of the exercises and the assessment of the students' performance are explained with the aid of three examples.

Keywords: mass and heat transfer, chemical reactions, fluid mechanics, Comsol Multiphysics, education.

1. Introduction

Processes in Chemical Engineering and in other engineering disciplines are described by differential equations. Analytical solutions do exist only for special cases, for simple geometries and idealized conditions. The modern engineer needs numerical solutions for process and apparatus design.

Present day education of engineers has to teach on the one hand the basics of various disciplines including traditional solution methods and on the other hand the use of modern numerical solution methods.

Based on the course entitled "The Finite Element Method" in the Bachelor program we go more deeply into this field in our Master program "Verfahrenstechnik / Process Engineering". Three engineering courses deal with computational methods and include computer exercises:

- Computational Fluid Dynamics with CFX,
- Process Simulation,
- Transport Processes with Comsol Multiphysics.

The education in these courses is complemented by the course entitled "Numerics and Optimization".

For the course entitled "Transport Processes" its contents, organization and aim as well as the priorities of the exercises and the assessment of the students' performance are all described in the following sections - with the aid of three examples.

2. The Course entitled "Transport Processes"

This course consists of 4 hours of instruction per week: 2 hours of lecture and 2 hours of computer exercises. Topics are taken from the fields of heat and mass transfer, chemical reaction engineering and fluid dynamics:

- steady state heat conduction - in a fin for increasing heat emission and the accompanying heating of a pipe,
- isothermal pore diffusion to obtain the effectiveness factor of a catalyst particle with various shapes,
- non-isothermal pore diffusion with a combination of mass and heat transfer,
- transient processes of heating / cooling, e.g. the heating of a sphere and a one-sided fired wall or freezing of a piece of meat with a phase change,
- axial dispersion in chemical reactors, combined with the estimation of conversion,
- electrically heated metallic component combined with the heat emission,
- laminar flow of Newtonian fluid to compare with Hagen-Poiseuille and non-Newtonian fluid in a tube,
- flow and heat transfer over a step.

In particular the basic and the chemical engineering modules of Comsol Multiphysics are employed.

Three points are used for the assessment of the students' performance. The first part consists of the grades for the reports of about 10 computer exercises. The students have to finish the calculations and present and discuss the results in a short paper. The second part of the assessment is the grade for the written final exam, which focuses on the basics of transport phenomena and of numerical solutions. The final part of the assessment is a grade for the individual homework assignment presented in the form of a paper and a Power Point presentation. Each student selects a special problem from a provided list, collects data and solves the problem on his own.

3. Aim of Learning / Methodical Concept

The methodical concept of the course concentrates on the following priorities:

1) At first very simple examples are solved with basic geometry under idealized conditions. This allows for analytical solutions - with pencil and paper or with the help math and engineering software entitled MAPLE. These analytical solutions can be compared with the results of FEM calculations (Comsol Multiphysics) and with the results of simple numerical methods (EULER method with EXCEL).

All possibilities are employed for the verification of the numerical results - e.g. the comparison between the subdomain integral over the reaction rate and the boundary integral over the mass or heat flux.

2) Based on the simple examples students progress to slightly more complicated geometries or conditions. On the one hand, that shows the path to the solution of practical problems. On the other hand it allows students to see the influence of simplifications / idealizations and to assess approximation formulas from literature. Such simplifications may concern the isolation of parts of surface, the plug flow in reactors or heat exchangers or the flow behavior of a Bingham substance.

Interestingly the simplifications necessary for analytical solutions may be a serious barrier for the numerical solution with finite element methods.

3) Each example is used to teach new aspects of modeling in Comsol Multiphysics in particular regarding steady state and transient calculations, the import of geometry, the use of data tables for properties of materials, the change of phase as well as other aspects.

4) Alternatives are discussed for description of problems: use of the axial dispersion model instead of the solution of the flow problem or the use of different geometries (1D, 2D, 3D, use of symmetry).

5) One aim of learning in this course concerns finding the similarities between various processes. For example, heat transfer in a fin without a source term is described by the same differential equation that applies to a first order chemical reaction in a catalyst plate.

6) Different results are obtained through variation of the number of elements. There is discussion on the accuracy of calculations depending on the number of elements. The dependence on element size can be compared with the influence of element size in the Euler or Runge-Kutta method.

4. Examples

4.1 Overview

Two kinds of examples are employed: very simple examples for comparison with analytical solutions and slightly more complicated examples. The simple examples are concerned with heat conduction in a fin, with isothermal pore diffusion in a plate or a sphere, with axial dispersion in chemical reactors, with laminar flow of Newtonian fluid in a tube or with the transient processes of heating / cooling of simple geometries.

The second kind of examples uses slightly more complicated geometries or conditions. These examples might be the completion of the listed simple examples - accompanying heating of a pipe, pore diffusion in different geometries or the freezing of meat with phase change. Examples are also used from the Comsol Multiphysics model library, e. g. the flow with heat transfer over a step or the electrically heated metallic component.

4.2 Steady State Heat Conduction

The first example deals with heat conduction in a fin for increasing heat emission. The simplified energy balance takes into account the heat conduction in the direction of longitudinal axis and heat emission from the surface of the fin. This results in the following ordinary differential equation

$$T'' - m^2 \cdot T = 0$$

and as a solution

$$T(x) = T_o \frac{\cosh(m(L-x))}{\cosh(mL)}$$

Through differentiation the following heat flux at position x is obtained from this equation for temperature:

$$\dot{Q}(x) = \lambda \cdot A \cdot T_o \cdot m \cdot \frac{\sinh(m(L-x))}{\cosh(mL)}$$

$$\dot{Q}_{all} = \dot{Q}(x=0) = \lambda \cdot A \cdot T_o \cdot m \cdot \tanh(mL)$$

For $x = 0$ it is the heat flux which is fed to the fin. Figure 1 shows the temperature and heat flux for one example.

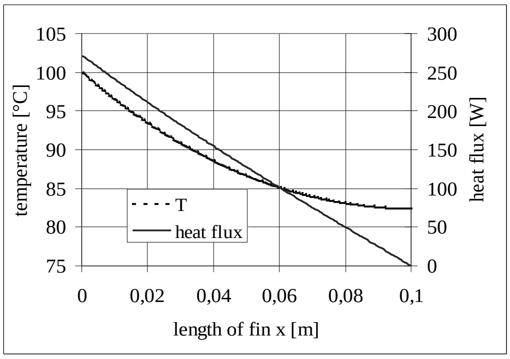

Figure 1. Temperature and heat flux depending on the length of fin.

A slightly more complicated example concerns the accompanying heating of a pipe. The students have to prepare the technical drawing with a CAD program. Then this "geometry" can be imported. The next steps concern the transformation to a solid and the conversion of millimeters to meters. The temperature field can be calculated for given values of heat convection coefficients, heat conduction coefficients, fluid temperatures in both pipes and the ambient temperature.

Figure 2 shows the temperature field for the given situation. The large pipe contains the product and the small pipe the heating fluid. Minimum and maximum temperatures and the amount of heat loss can be obtained based on these results.

The next step concerns optimization that means the minimization of heat consumption for maintaining the required product temperature.

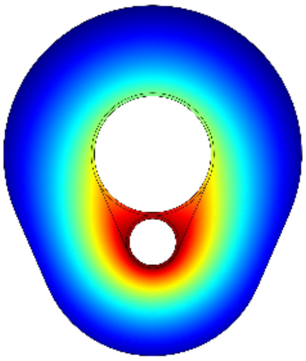

Figure 2. Temperature field of the accompanying heating of a pipe.

4.3 Diffusion in Heterogeneous Catalysts

For the first order reaction in a heterogeneous catalyst plate with diffusion transport and consumption by a chemical reaction the same mathematical equation can be obtained as above for the heat transport in a fin. C is the dimensionless concentration of the reaction component, X the dimensionless coordinate and ϕ_L is the Thiele modulus for the plate and a first order reaction.

$$C'' - \phi_L^2 \cdot C = 0$$

$$C(X) = \frac{c}{c_K} = \frac{\cosh(\phi_L X)}{\cosh(\phi_L)}$$

$$\phi_L^2 = L^2 \cdot \frac{k}{D_{eff}}$$

For the estimation of the catalyst effectiveness factor there are two possible ways to obtain the calculation of the converted amount (by way of analytical solution and similarly by way of the numerical solution). The first way is the subdomain integration over the reaction rate (source term).

$$\eta = \frac{\int_0^{V_K} k \cdot c(x) \cdot dV_K}{k \cdot c_K \cdot V}$$

The following second way concerns the calculation of the diffusion flux at the boundary of the plate.

$$\eta = \frac{\dot{n}_{Diff}}{k \cdot c_K \cdot V}$$

In either case the following formula is obtained from the analytical solution

$$\eta = \frac{\tanh(\phi_L)}{\phi_L}$$

A modified Thiele modulus allows for the comparison of different geometries. Instead of diameter or height the ratio of volume and outer surface is employed. For plates there is no difference: $L = V/O$ and $\phi_L = \phi_{mod}$

$$\phi_{mod}^2 = \left(\frac{V}{O}\right)^2 \cdot \frac{k}{D_{eff}}$$

Figure 3 shows the effectiveness factor depending on the Thiele modulus for different shapes of catalyst. The greatest difference between sphere and plate of about 14% is found at $\phi_{mod} =$ 1.5. This includes the results of calculations with Comsol Multiphysics for a cylinder ($h = d$), a hollow cylinder ($h = d = 2\,d_i$) and a monolithic catalyst with rectangular canals.

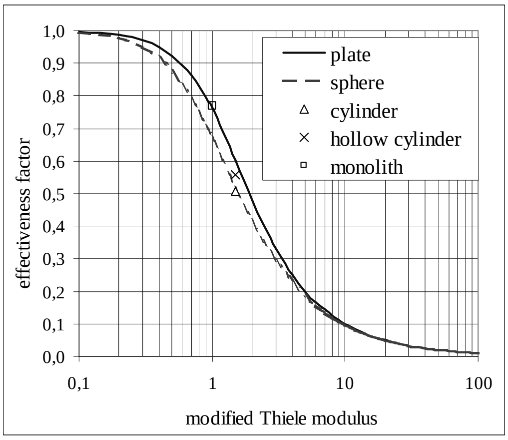

Figure 3. Effectiveness factor depending on the Thiele modulus.

For the case of a sphere catalyst particle the students have to calculate the concentration profile for a first order reaction with the Euler method while using Excel. From

$$C'' + \frac{2}{X} \cdot C' - \phi_S^2 \cdot C = 0$$

a system is obtained with two ordinary differential equations.

$$C' = Z$$

$$Z' = -\frac{2}{X} \cdot Z + \phi_S^2 \cdot C$$

For a given value of ΔX there is a difference between numerical and analytical solution. Figure 4 shows the error in calculation, that means the above-mentioned difference between analytical and numerical solution for the concentration at X = 1 depending on the step size. The method employed is based on the following formula.

$$C_1, Z_1 = f(X_o, C_o, Z_o)$$

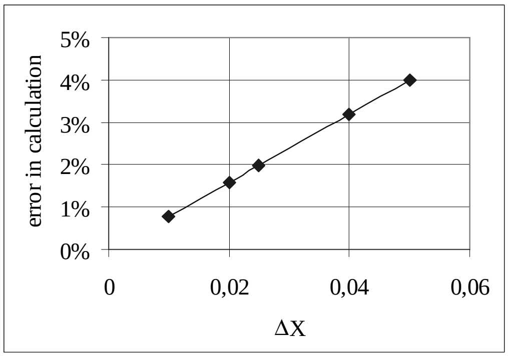

Figure 4. Error in calculation (concentration difference) at X = 1

In the case of exothermic reactions it is possible, that the catalyst effectiveness factor is greater than 1. This is due to the enhancement of the chemical reaction by the higher temperature inside the catalyst particle. Analytical solutions do not exist.

Figure 5 shows calculated results exemplary for the decomposition of nitrogen oxide (N_2O). The interaction between the temperature and concentration fields causes a thin layer with a high reaction rate. For a lower radius the temperature is high, but the concentration of the reactant is nearly zero. And for a greater radius the concentration is high, but the temperature is not sufficient for the start of chemical reaction.

In this case there is an effectiveness factor of $\eta = 13.3$! That means that the reaction rate is about 13 times faster compared with the case of neglecting of all transport resistances (equivalent to a reaction rate under surface conditions). The comparison of the calculated data with data reported in literature indicates good agreement.

An indication of the quality of the calculations can be determined by using the combination of energy and mass balances. This combination results in the Prater number β:

$$\beta = \frac{T_o - T_S}{T_S} = \frac{(-\Delta H) \cdot D_{eff} \cdot c_S}{\lambda_{eff} \cdot T_S}$$

The same numerical value is obtained in the above-mentioned example by using the difference between the surface and center temperature as well as by using the properties and the surface concentration.

The difficulties in numerical calculation are due to the possible existence of very high gradients. That is why we have to start with very low surface concentrations. Then the concentration can be increased step by step. Alternatively the parametric calculation method can be used.

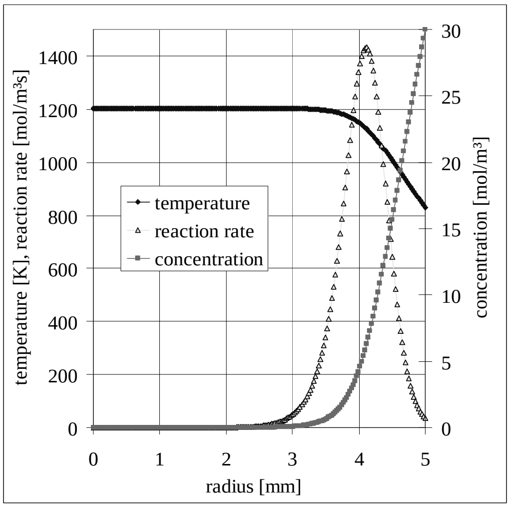

Figure 5. Temperature, concentration and reaction rate depending on radius of a spherical catalyst particle.

4.4 Transient Heating of a Wall

"Transient heating" is an important process in many application fields: from heating / cooling of work pieces to cooking / freezing of food. Analytical solutions exist only for special cases. They consist of an infinite sum of partial functions. Simple functions are obtained only for very short or very long periods of time.

The selected example concerns the one-sided heating of a wall. The practical background could be a fired wall of a store-room. How rapidly does the temperature of the cold side of the wall increase? An analytical solution exists for the case of adiabatic behavior of the cold side. With Comsol Multiphysics the solutions can be compared for the adiabatic behavior and for the case of convective heat transfer to the cold environment. Figure 6 shows the temperature of the cold side of the wall depending on the time for both variants. "Convective" means convective heat transfer to the cold environment (20°C) with a heat transfer coefficient of 20 W/m²K.

In postprocessing the heat flux can be obtained at both boundaries - hot and cold - depending on time. Figure 7 shows these data. The absorbed heat flux at the start of the heating process is very high and the gradient is high as well.

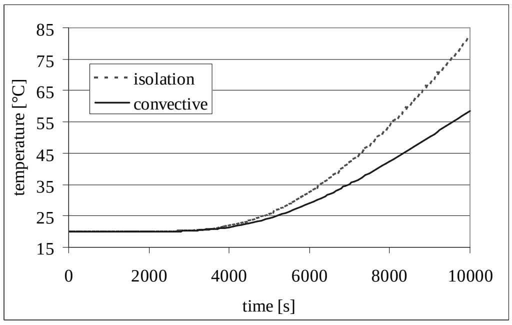

Figure 6. Temperature of the cold side of the wall depending on time.

These data can be exported to Excel and then calculated for the difference between both heat fluxes (input and output). The integration of this flux difference over time with the Simpson method results in the accumulated energy inside the wall.

$$Q(t) = A \cdot \int_0^t \left(\frac{\Delta \dot{Q}}{A} \right) dt$$

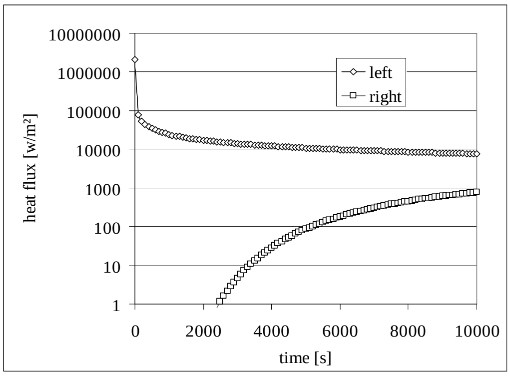

Figure 7. Heat flux at both boundaries

On the other hand this result (the accumulated energy) is obtained through comparison of the initial temperature and mean temperature at time *t*. The mean temperature is obtained by subdomain integration over *T(x)* for a given time.

$$\overline{T} = \frac{1}{V} \cdot \int T dV$$

$$Q(t) = m \cdot c \cdot (\overline{T}(t) - T_o) = V \cdot \rho \cdot c \cdot (\overline{T}(t) - T_o)$$

For our data shown in figures 6 and 7 there is a difference of about 30%. This is due to the extremely high gradient of heat flux in the first seconds. This provides a good starting point for a discussion with students. What influence does the subdivision in elements have on the accuracy of results? Which differences can be tolerated?

5. Conclusions

The aim of the course entitled "Transport processes" is to deepen and consolidate the students' knowledge in the fields of heat and mass transfer, chemical reaction engineering and fluid dynamics. This should be combined with education in the field of numerical calculation of various processes. Comsol Multiphysics is a very useful instrument to reach this aim. Even the problems linked to finite element calculations help students to understand processes as well as solution methods.

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