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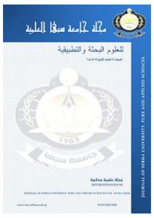

Analysis Approach Development of Transport Phenomena for Engineers in Industry: basic concepts and advanced solving techniques

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ABSTRACT

Applied Mathematical representation Phenomena Sciences in Engineering development is related to the knowledge advances of different areas of Chemical Engineering and other engineering fields. The advances in mathematical analysis and the computer tools in Transport Phenomena help solve complex problems involving momentum, heat, and mass transfer. Transport Phenomena applied to the engineering teaching process presents unique challenges regarding the complexity of biological material and how it changes during the application of different transformation or preservation treatments. Therefore, studying the basic concepts of Transport Phenomena and their applications to analyze, predict, and design any process is essential in advancing industrial Engineering. This paper presents some of those fundamental concepts of recent applications and research orientations. Several critical elements of numerical analysis are profiled in COMSOL Multiphysics with 0-D, 1-D, 2-D, and 3D models. These elements are root-finding, ordinary and partial differential equations, and linear system analysis. These methods underly nearly all problem-solving techniques by numerical analysis for chemical engineering applications. COMSOL Multiphysics is illustrated concerning some typical applications in chemical engineering.

تطوير أسس تحليل ظواهر الانتقال للمهندسين في الصناعة: المفاهيم الأساسية وتقنيات الحل المتقدمة

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الملخص

يرتبط علم ظواهر التمثيل الرياضي التطبيقي في التطوير الهندسي بالتقدم المعرفي لمجالات مختلفة من الهندسة الكيميائية والمجالات الهندسية الأخرى. واحدة من هذه المجالات هي ظواهر الانتقال، وبيان مدى التقدم بالتحليل الرياضي والاستخدام الأمثل لأدوات الحاسوب التي تساعد في حل المشاكل المعقدة التي تنطوي على انتقال الموائع والحرارة وانتقال الكتلة. تعاني طرق تحليل ظواهر الانتقال المطبقة في عملية تدريس مقررات الهندسة تحديات خاصة فيما يتعلق بتعقيد المواد البيولوجية وكيف تتغير أثناء تطبيق معالجات التحول أو الحفظ المختلفة. تعتبر دراسة المفاهيم الأساسية لظواهر الانتقال وتطبيقاتها لتحليل أي عملية والتنبؤ بها وتصميمها خطوة مهمة في تقدم الهندسة الصناعية. يتم تقديم بعض هذه المفاهيم الأساسية والأمثلة للتطبيقات الحديثة وتوجهاتها

الكلمات المفتاحية:
الرياضيات التطبيقية
التطوير الهندسي
ظواهر الانتقال الهندسي
التصميم بمساعدة الحاسوب
تطبيق متعدد الفيزياء (COMSOL).

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البحثية في هذه الورقة. تم تحديد العديد من العناصر الرئيسية للتحليل العددي باستخدام تطبيق متعدد الفيزياء (COMSOL) مع نماذج D , 1-D , 2-D-0، وأيضا D-3 ومن هذه العناصر هي إيجاد الجذر، التكامل العددي، المعادلات التفاضلية العادية، وتحليل النظام الخطي. هذه الطرق هي أساس جميع تقنيات حل المشكلات تقريبًا عن طريق التحليل العددي لتطبيقات الهندسة الكيميائية. تم توضيح استخدام هذه الطرق في برنامج كومسول بالرجوع إلى بعض التطبيقات الشائعة في الهندسة الكيميائية: التقطير الوميضي، وتصميم المفاعل الأنبوبي، والأنظمة التفاعلية، والتوصيل الحراري في المواد الصلبة.

Introduction

Engineering alumni are confronting an arising class of configuration challenges with different controls of science and innovation. Modern computational methods, joining the delegate physical science of numerous areas, are expected to show and foresee results precisely. Most engineering degree programs offer major-specific modelling courses or embed simulations on a limited basis. For example, chemical engineering graduate students may be exposed to mass and heat modelling and computational fluid dynamics problems. Few engineering curricula, including those in our department, offer multi-physics design and research experiences. Where available, they are typically restricted to some term projects for postgraduate studies; consequently, most main graduate course curricula have little or no exposure to areas of expertise outside their discipline. That is inconsistent with the view that future graduates need to be more adaptable and versatile to succeed in the global marketplace [1]. Many similarities exist in the chemical and biological processing industries in entering materials to get into the final chemical. Those chemicals are separated through steps called unit operations. However, in Chemical Engineering, the term "unit operations" has largely been superseded by the current and descriptive term "separation processes" [2]. These processes have fundamental principles such as diffusion, and mass transfer occurs in the drying of foods, gas transfer in flexible packages. Transport phenomena are the term of dominating these processes. It is also thought to be an essential link between the processing of these resources and the product's quality and safety. The bioengineering industries are still dominated by empiricism or so-called pragmatic approaches. Possible reasons for this situation are (1) Transport phenomena mathematical derivations and solutions are poorly understood, due to difficult mathematical solutions analytically. (2) Even when fully understood, classical transport phenomena theory is difficult to apply to biological materials due to their unique structure and features. (3) Individuals working in the industry are not convinced of the importance of transport phenomena, possibly because of how universities teach the subject [2]. Other factors must be considered in addition to these reasons when applying traditional transport phenomena notions to industrial Process Engineering. The requirement for specific transport properties for a variety of industrial materials and new products, as well as an understanding of new technologies and their link to the transfer phenomena to be used in each case, and the production of specific transport qualities. In this paper, some fundamental ideas of transport phenomena and instances of the current circumstance of utilizations and examination in Engineering are presented. The authors have created a short course for Engineers and Scientists, senior undergraduates and graduates focused on the methods and techniques used in multidisciplinary modelling. Contextualized assignments are selected from high-priority research topics. A broad recognition believes that meaningful learning in engineering requires that students master fundamental concepts rather than memorizing facts and formulas [3- 4]. Deeper understanding and a smoother transfer to other domains of contextualized projects lead to a more enjoyable experience motivating Engineers and Scientists to work in a new way.

Numerical Methods for Engineers

The modules created using this new approach enable students to work through Exercises that progress from fundamental ideas and concepts to more complicated circumstances where critical thinking and creativity are encouraged.

The numerical engine for simulating multiple system components involving fluid flow, heat transfer, and species transport were chosen as COMSOL Multiphysics. A library of numerous models was also built to allow researchers to investigate the impact of various model parameters on the physical system without worrying about numerical solution specifics. This method will enable them to concentrate on gaining a more profound knowledge of system physics, which helps to reinforce the foundations taught in mandatory fluid mechanics, heat transfer, and mass transfer courses. To provide a more direct connection between the model equations and the calculated results, a Graphical User Interface (GUI) was created using COMSOL that provides either a 0-D, 1-D, 2-D, and 3-D visualization of the model simulations where the effect of various model parameters can be explored [5].

One approach uses numerical techniques in which the physical geometry is represented by a mesh of finite elements that collectively satisfy the relevant equations. The preferred approach is to employ a single solution builder to configure, constrain, solve, and post-process results. At times, multiple models, each with specific geometry, materials, constraints, and physics, may be used sequentially or co-exist and be coupled. As with all numerical methods, care must be taken to ensure proper convergence and accuracy of the result. Model creation typically proceeds along these lines: define problem steps, including simplifying assumptions, identify global constants and expressions, construct physical geometry including symmetries, and specify domains and material properties. In addition, other efforts are needed to get model results, such as setting boundary conditions, meshing physical structure into finite elements, selecting physics for each domain, configuring study types, initiating solver, and post-processing results for more visualized forms.

Multiphysics software COMSOL can accelerate the timetable needed to create a working model. A family of graphical interfaces, organized in a tree structure, guides the development process while providing contextual help along the way. A properties library is embedded that covers many common materials. Meshing options include external file import and adaptive techniques where dynamic adjustments are made during the solving process. If necessary, users customize the physics further by adding additional algebraic expressions and partial differential equations. This analysis approach philosophy paper has based their findings and discussions on their published work throughout the teaching process for the last several years. The authors used COMSOL Multiphysics software and its new Apps application builder features throughout the teaching process in the heat transfer course by Edali et al. [6]. The transport phenomena course by Sahem et al. [7] and the fluid mechanics course by Edali et al. [8] are other works to achieve the main goals, maximizing the learning process's efficiency. Edali et al. [9] found that in Engineering based courses, using simulation apps are helping to expand the investigation techniques while keeping students engaged in striking such a balance by introducing students to complex concepts in a simplified format.

Solving nonlinear algebraic equations.

Consider the chemical equilibrium problem posed in the following equation, which governs the water-gas shift reaction [10].

$$CO + H_2O <=> CO_2 + H_2 \qquad (1)$$

That can be used in a chemical process to make hydrogen for fuel cell applications; the equation at equilibrium [10] must be solved.

$$K = (yCO_2\ yH_2) / (yCO\ yH_2O) \qquad (2)$$

Thermodynamic data give the value of ($K = 148.4$) at 500 K. If you start with a stoichiometric mixture of carbon monoxide and water. The equilibrium composition, in this case, can be the number of moles that remain the same when the reaction takes place. So the equation becomes with a basis of 1 mol each of carbon monoxide and water, which then react to equilibrium, and using x to represent the number of moles reacting, the equation that must be solved is.

$$f(x) = 148.4 - \frac{x^2}{(1-x)^2} = 0 \qquad (3)$$

While this can easily be solved by taking the square root and solving a linear equation, we solve it 'as is'; the method applies to more complicated problems that don't have an easy solution.

COMSOL Multiphysics, as shown in figure 1 at 0-D option, can be used under Mathematics-ODE and DAE Interface, typing in 'x' for the name and (148.4 - (x^2)/(1-x) ^2) for the f.

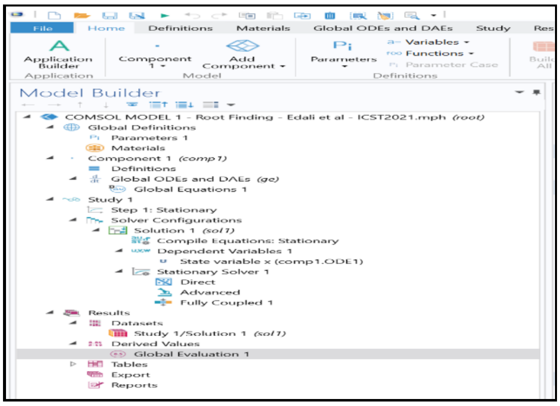
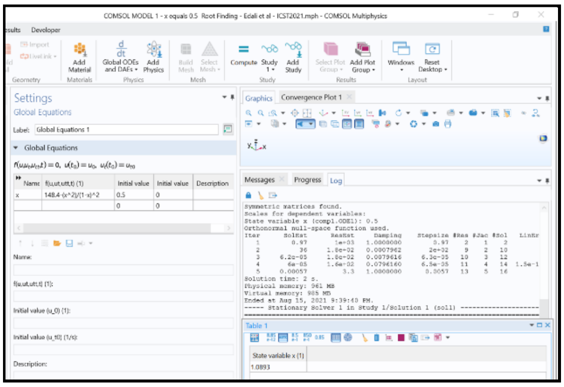


Fig. 1: COMSOL 0_D Model Global ODEs and DAEs (ge) solving a nonlinear algebraic equation.

Inserting 0.5 for the initial value and Clicking on Study 1 and choose Compute. If you look at the log, you see that the SolEst goes from about 0.97 to 5.7e-4 in 5 iterations. On the Results arrow on open Derived Values were listed there is State variable x, by clicking 'Evaluate' in the Global Evaluate window will give the result. A new column is formed labelled as 'State variable 'x', and the answer is 1.0893. The solution produced in Figure 2, should never be above 1.0, since x represents the number of moles of carbon monoxide reacting and the total available is 1.0.



Label: Global Equations 1

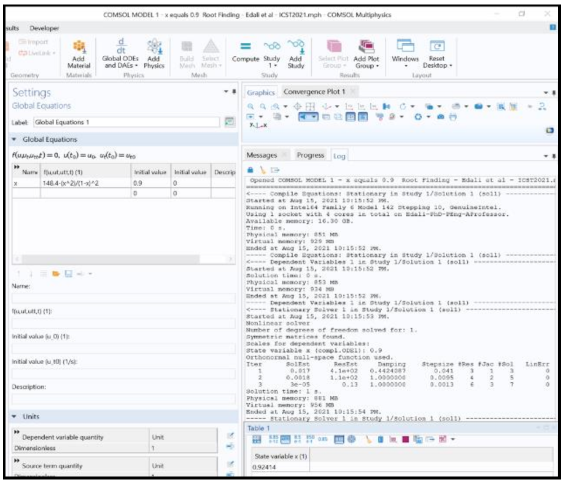
Name	f(u,ut,utt,t) (1)	Initial value (u_0) (1)	Initial value (u_t0) (1/s)	Description
x	148.4-(x^2)/(1-x)^2	0.5	0	

```
Symmetric matrices found.
Scales for dependent variables:
State variable x (comp1.ODE1): 0.5
Orthonormal null-space function used.
Iter      SolEst     ResEst     Damping    Stepsize #Res #Jac #Sol   LinEr
   1        0.97      1e+03   1.0000000       0.97    2    1    2
   2          36    1.8e+02   0.0007962     2e+02    9    2   10
   3     6.2e-05    1.8e+02   0.0079616    6.3e-05   10    3   12
   4       6e-05    1.6e+02   0.0796160    6.5e-05   11    4   14  1.5e-1
   5     0.00057        3.3   1.0000000     0.0057   13    5   16
Solution time: 2 s.
Physical memory: 961 MB
Virtual memory: 985 MB
Ended at Aug 15, 2021 9:39:40 PM.
----- Stationary Solver 1 in Study 1/Solution 1 (sol1) -------------------
```

State variable x (1)
1.0893

Fig. 2: COMSOL 0_D Model solution analysis at initial value x=0.5 for water-gas shift reaction governing equation.

Something is wrong where most nonlinear algebraic equations have more than one solution, and the solution obtained depends upon the initial guess. Go back to Global Equations in Figure 3 and change the initial guess to 0.9; right-click on the study and solve the problem again. To browse the new Results, the = sign is to be clicked on the Derived Values, State variable. The Results Table lists 0.92414, which is the accurate right solution found in other old, complicated solution techniques.



Label: Global Equations 1

Name	f(u,ut,utt,t) (1)	Initial value (u_0) (1)	Initial value (u_t0) (1/s)	Descrip
x	148.4-(x^2)/(1-x)^2	0.9	0	

```
Opened COMSOL MODEL 1 - x equals 0.9  Root Finding - Edali et al - ICST2021.
==========================================================================
<---- Compile Equations: Stationary in Study 1/Solution 1 (sol1) ----------
Started at Aug 15, 2021 10:15:52 PM.
Running on Intel64 Family 6 Model 142 Stepping 10, GenuineIntel.
Using 1 socket with 4 cores in total on Edali-PhD-PEng-AProfessor.
Available memory: 16.30 GB.
Time: 0 s.
Physical memory: 851 MB
Virtual memory: 929 MB
Ended at Aug 15, 2021 10:15:52 PM.
----- Compile Equations: Stationary in Study 1/Solution 1 (sol1) ----------
<---- Dependent Variables 1 in Study 1/Solution 1 (sol1) ------------------
Started at Aug 15, 2021 10:15:52 PM.
Solution time: 0 s.
Physical memory: 853 MB
Virtual memory: 934 MB
Ended at Aug 15, 2021 10:15:52 PM.
----- Dependent Variables 1 in Study 1/Solution 1 (sol1) ------------------
<---- Stationary Solver 1 in Study 1/Solution 1 (sol1) --------------------
Started at Aug 15, 2021 10:15:53 PM.
Nonlinear solver
Number of degrees of freedom solved for: 1.
Symmetric matrices found.
Scales for dependent variables:
State variable x (comp1.ODE1): 0.9
Orthonormal null-space function used.
Iter      SolEst     ResEst     Damping    Stepsize #Res #Jac #Sol   LinErr
   1       0.017    4.1e+02   0.4424087      0.041    3    1    3        0
   2      0.0018    1.1e+02   1.0000000     0.0095    4    2    5        0
   3       3e-05       0.13   1.0000000     0.0013    6    3    7        0
Solution time: 1 s.
Physical memory: 881 MB
Virtual memory: 956 MB
Ended at Aug 15, 2021 10:15:54 PM.
----- Stationary Solver 1 in Study 1/Solution 1 (sol1) --------------------
```

Dependent variable quantity	Unit
Dimensionless	1

State variable x (1)
0.92414

Fig. 3: COMSOL 0_D Model solution analysis at initial value x=0.9 for water-gas shift reaction governing equation.

Transport and Transfer processes

Engineering processes involve the transport and transfer of mass, energy, and momentum. The Mass transfer consists of separating a mixture of chemicals into separate streams, possibly nearly pure streams of one component. Energy transfer is used to heat reacting streams, cool products, and run distillation columns. Momentum transfer is another word for fluid flow, and most chemical processes involve pumps, compressors, and perhaps centrifuges and cyclone separators.

These subjects were unified in 1960 in the first edition of the classic book, Transport Phenomena (Bird et al., 2002). Such transport problems are solved in one-dimensional; the solution is a function of one spatial dimension. The one-dimensional problems lead to differential equations, which are solved using the latest version of COMSOL (5.6). Diffusion problems in one dimension led to boundary value problems (BVP). As boundary conditions are applied at two different spatial locations, one side is the concentration may be fixed, and the flux may be fixed on the other side. Because the conditions are specified at two different locations, the problems are not initial values in character. It is impossible to begin at one position and integrate directly because at least one of the conditions is specified somewhere else. Thus, there are not enough conditions to start the calculation. One can notice the equations governing mass transfer as diffusion across a flat slap as in equation 4, energy transfer as steady heat conduction transfer across a slab as in equation 5, and fluid flow as the flow of a Newtonian fluid in a pipe, as in equation 6.

The concentration, c, in equation 4 is a function of position, x. The diffusivity, D, can depend upon concentration [10]. This is also a two-point boundary value problem because the concentration is specified at x = 0 and x = L.

$$\frac{d}{dx}\left(D\,\frac{dc}{dx}\right) = 0 \qquad (4)$$

$$C(0) = c_0\,,\ c(L) = c_L$$

The temperature, T, in equation 5 is a function of position, x [10]. That one condition is at x = 0 and the other is at x = L. This makes it a two-point boundary value problem. The problem is nonlinear when the thermal conductivity k depends upon temperature and when it does. The rate of energy generation is Q.

$$\frac{d}{dx}\left(k(T)\,\frac{dT}{dx}\right) = Q \quad (5)$$

$$T(0) = T_0\,,\ T(L) = T_L$$

A governing differential equation can describe the flow of a Newtonian fluid in a pipe, as in equation 6 [10]. The r is the radial position from the center of the conduit of radius R, v is the velocity in the axial direction, m is the viscosity, Δp is the pressure drop along the pipe, and L is the length over which the pressure drop occurs. The boundary conditions are at different locations, making it a two-point boundary value problem.

$$\frac{1}{r}\frac{d}{dr}\left(r\mu\,\frac{dv}{dr}\right) = -\frac{\Delta p}{L} \qquad (6)$$

$$\frac{dv}{dr}(0) = 0, \qquad v(R) = 0$$

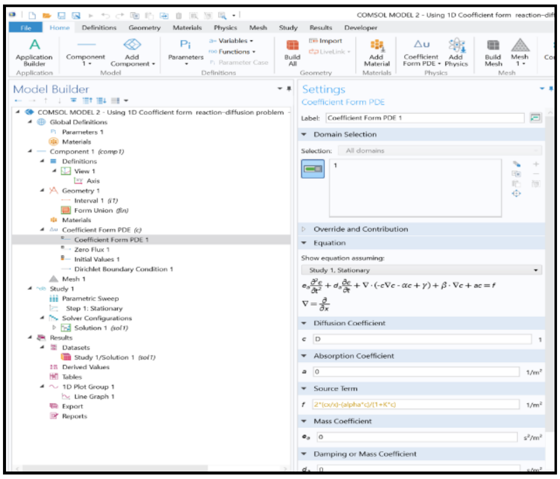
When the fluid is non-Newtonian, it may not be possible to solve the problem analytically. The viscosity depends upon the shear rate, dv/dr. For problems like this, numerical methods must be used.

The following is the solution to the reaction-diffusion problem in a spherical domain [10] using COMSOL Multiphysics tools, as shown in figure 4. The reaction rate expression is a nonlinear function of concentration, appropriate for the Michaelis–Menten reaction in biological systems. The non-dimensional form of the problem is shown in equation 7 [10], and it is solved for α= 5, K = 2.

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2\,\frac{dc}{dr}\right)=\frac{\alpha c}{1+Kc} \qquad (7)$$

$$\left(\frac{dc}{dr}\right)(0)=0, \qquad c(1)=1$$

COMSOL was used in a Coefficient form 1-D PDE with Dirichlet boundary conditions mode with one dependent variable.



Coefficient Form PDE

Label: Coefficient Form PDE 1

Domain Selection

Selection: All domains

1

Override and Contribution

Equation

Show equation assuming:

Study 1, Stationary

$$e_a\frac{\partial^2 c}{\partial t^2}+d_a\frac{\partial c}{\partial t}+\nabla\cdot(-c\nabla c-\alpha c+\gamma)+\beta\cdot\nabla c+ac=f$$

$$\nabla=\frac{\partial}{\partial x}$$

Diffusion Coefficient

c: D (1)

Absorption Coefficient

a: 0 (1/m²)

Source Term

f: 2*(cx/x)-(alpha*c)/(1+K*c) (1/m²)

Mass Coefficient

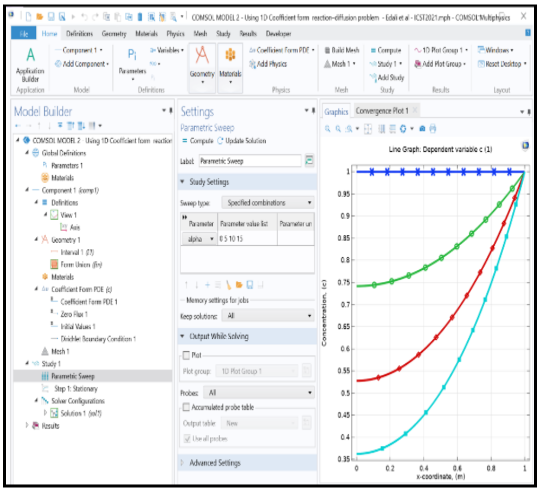
e_a: 0 (s²/m²)

Damping or Mass Coefficient

d_a: 0

Fig. 4: COMSOL 1_D Model Coefficient Form setting.

The Parametric solution is instructive to solve this problem for multiple parameters, α, which can be done in COMSOL using the parametric solver. In Physics/Subdomain Selection, the used variable name, alpha, in Physics/Subdomain Selection, would be set at several values. The program solves the problem for a variety of alphas. Figure 5 indicates that the concentration decreases from the outer part of the sphere to the inner part of the sphere and that this decrease is more dramatic with larger values of alpha. This is because the reaction rate is faster, and diffusion cannot keep up, thus decreasing the concentration. Figure 5 also shows the rate of reaction as a function of position and alpha.



Parametric Sweep

Compute | Update Solution

Label: Parametric Sweep

Study Settings

Sweep type: Specified combinations

Parameter	Parameter value list	Parameter un
alpha	0 5 10 15	

Memory settings for jobs

Keep solutions: All

Output While Solving

☐ Plot

Plot group: 1D Plot Group 1

Probes: All

☐ Accumulated probe table

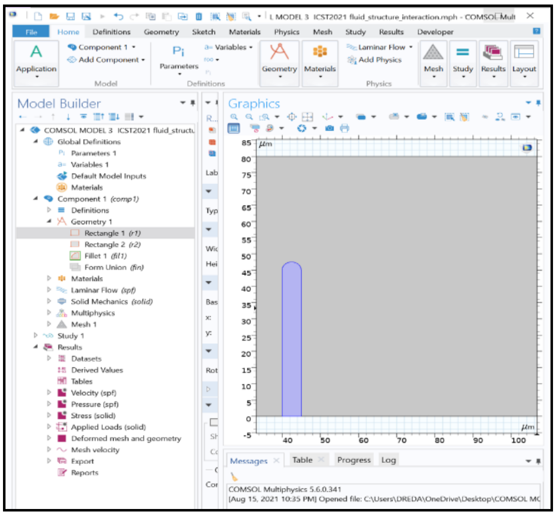
Output table: New

☑ Use all probes

Advanced Settings

Fig. 5: COMSOL 1_D Model, Concentration in spherical domain with Michaelis–Menten reaction.

The last model for this paper demonstrates how to set up a fluid-structure interaction (FSI) problem in COMSOL Multiphysics. The model geometry in Figure 6 consists of a horizontal flow channel in the middle of which is an obstacle, a narrow vertical structure. Elastic formulation and a nonlinear geometry formulation were used to solve for the structural deformations to allow large deformations. Finally, the flow was let to flow over the obstacle, which was fixed to the bottom of the fluid channel.

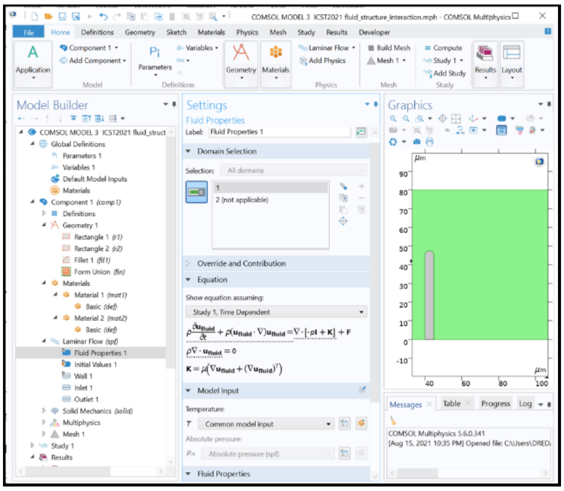


COMSOL Multiphysics 5.6.0.341

[Aug 15, 2021 10:35 PM] Opened file: C:\Users\DREDA\OneDrive\Desktop\COMSOL MC

Fig. 6: COMSOL 2_D Model, the fluid flow in a deformed, moving mesh that follows the movement of the bending structure.

The fluid is a water with a density ρ = 1000 kg/m3 and dynamic viscosity η = 0.001 Pa·s. The structure consists of flexible material with a density ρ = 7850 kg/m3 and young's modulus *E* = 200 kPa. Flow in the channel is described in figure 7 by the incompressible Navier-Stokes equations for the velocity field, **u** = (*u*, *v*), and the pressure, *p*, in the spatial deformed as a moving coordinate system.



Fluid Properties

Label: Fluid Properties 1

Domain Selection

Selection: All domains

1

2 (not applicable)

Override and Contribution

Equation

Show equation assuming:

Study 1, Time Dependent

$$\rho\frac{\partial \mathbf{u}_{\mathrm{fluid}}}{\partial t}+\rho(\mathbf{u}_{\mathrm{fluid}}\cdot\nabla)\mathbf{u}_{\mathrm{fluid}}=\nabla\cdot[-p\mathbf{I}+\mathbf{K}]+\mathbf{F}$$

$$\rho\nabla\cdot\mathbf{u}_{\mathrm{fluid}}=0$$

$$\mathbf{K}=\mu\left(\nabla\mathbf{u}_{\mathrm{fluid}}+(\nabla\mathbf{u}_{\mathrm{fluid}})^T\right)$$

Model Input

Temperature:

T: Common model input

Absolute pressure:

p_A: Absolute pressure (spf)

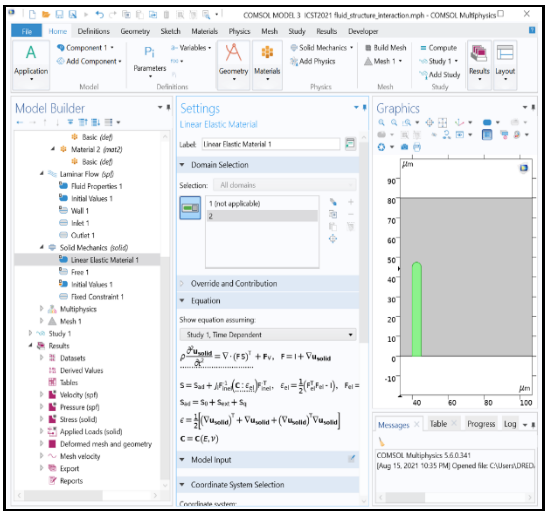
Fluid Properties

COMSOL Multiphysics 5.6.0.341

[Aug 15, 2021 10:35 PM] Opened file: C:\Users\DRED/

Fig. 7: COMSOL 2_D Model, the fluid flow in a deformed, moving mesh that follows the movement of the bending structure.

The obstacle forces the fluid flowing from left to right into a narrow path in the upper part of the channel. In addition, it imposes a force on the structure's walls resulting from the viscous drag and fluid pressure, as shown in figure 8.



COMSOL Multiphysics 5.6.0.341
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Fig. 8: COMSOL 2_D Model, Solid Mechanics Interface with the Laminar Flow.

The solid and the fluid, respectively, were modelled by a Solid Mechanics interface with a Single-Phase Flow interface model. FSI couplings coupled the boundaries between the fluid and the solid. The Fluid-Structure Interaction interface was modelled using an arbitrary Lagrangian-Eulerian (ALE) approach. It was to combine the fluid flow described by an Eulerian model. A Lagrangian description and a material frame were used to create a spatial frame with solid mechanics. The structure, made of a deformable material, bends under the applied load, as shown in Figures 8 and 9.

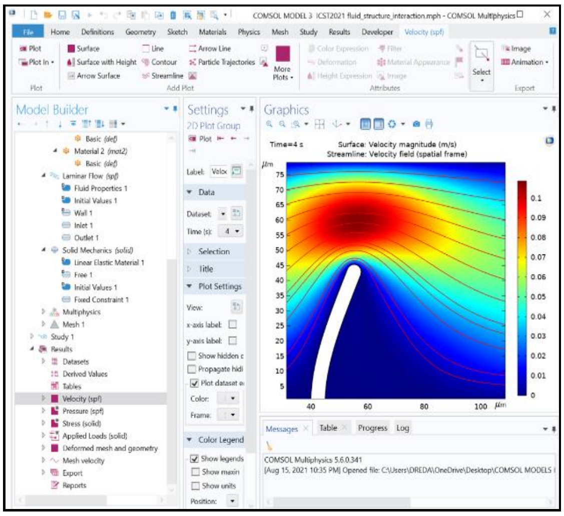

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Fig. 9: COMSOL 2_D Model, Flow velocity and geometry deformation at t = 4 s.

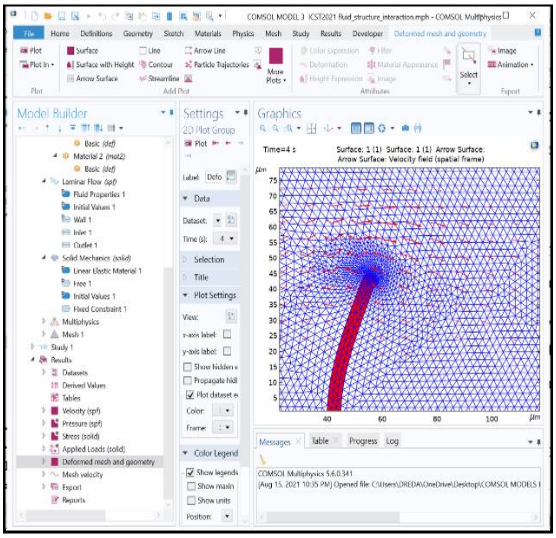

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Fig. 10: COMSOL 2_D Model, Mesh velocity (arrows) and mesh and geometry deformation at t = 4 s.

Conclusion

Many University professors would agree that transport phenomena are as challenging to teach as they are essential. Students, too, would agree that translating Fourier's law or Navier–Stokes's equations into a mental image of the flow patterns of heat and fluid in a system is no easy task. Most transport equations are nonlinear, comprising partial differential and integral equations that often involve complex coupled systems. The associated material properties are often a function of temperature, pressure, and several other parameters. Solving these transport Phenomena problems was usually done in the classroom using simplifications, including linearizing, approximating, and using accepted assumptions. These simplifications mean the solutions are, to some extent, erroneous. That technique is undoubtedly the best way of developing a basic understanding of solving numerical problems. COMSOL Multiphysics provides a powerful numerical platform where various industrial process technology components models can be readily created for education and research. The GUIs enable researchers to study the effect of various design parameters readily. These applications reduce the complexity of model setup and computational time and emphasize understanding Multiphysics in multi-dimensions that are otherwise impossible with simple 1-D models. Practical suggestions and references are concluded in short in this paper for implementing a unified strategy for teaching simply too advanced Transport Phenomena problems solutions. Finally, with only the efforts of staff, with a wide range of academic, industrial, and lab experience that mirrors engineers' wide-ranging background and experience, this analysis solving approach program can be achieved. Researchers will find it beneficial within future industrial needs.

Acknowledgment

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