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MODELING PAPER DRYING WITH COMSOL MULTIPHYSICS MODELING TOOL

Abstract

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Modeling Paper Drying with Comsol Multiphysics Modeling Tool, 42 pages, 4 appendices

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The main objective of our research was to develop a model with COMSOL Multiphysics modeling tool for paper drying process. We tried to simulate a model which could include all the physical phenomena during the paper drying process. With this model we could control the papermaking process in the paper mill to get good paper to meet the requirements of the clients. Besides, we could compare our results with the earlier study result carried out by other researchers. The work was commissioned by Esko Lahdenperä.

This study was carried out using COMSOL Multiphysics modeling tool. We did not need to concentrate on solving equations. We tried to build a model with COMSOL Multiphysics modeling tool. First we modeled a simple model of water vapor diffusion in base paper, then we added the heat transfer in paper, heat transfer from surface into air and mass transfer from surface into air to the first model. The rest work can be done in the same manner.

The COMSOL Multiphysics modeling tool is very helpful to study multiphysics phenomena. We have got more detailed understanding of modeling work, this tool and the phenomenon itself. What we have got is quite satisfying, even though there will be some problems. The stepwise work will still be continued.

Key words: model, COMSOL Multiphysics modeling tool, paper drying

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1 Introduction

Computer simulation has become an essential part of science and engineering. Digital analysis of components, in particular, is important when developing new products or optimizing designs. Modeling has a spectrum of applications which range from concept development and analysis, through experimentation, measurement and verification, to disposal analysis. Projects and programs may use hundreds of different simulations, simulators and model analysis tools.

Several previous studies on the drying process of base sheet paper and coated paper have been carried out, describing the heat and water transport with developing a mathematical model. The modeling work does not need to concentrate on the equation solving part and we can do our research in a much faster and more efficient way. Besides, we can compare our results with the previous experimental results. On one hand, the experiments can be verified which makes the result much more reliable, on the other hand, we can learn the phenomena efficiently.

The objective of the present investigation is to develop a model with COMSOL Multiphysics modeling tool for paper drying process. We try to simulate a model which can be used for simulation of the heat and mass transfer in paper web. Approximating equations concerning the paper properties are used in modeling process, but we don't need to develop the mathematical model because it has been developed in the COMSOL Multiphysics modeling tool which can lessen large quantities of calculation work.

The thesis includes two main sections: literature review and simulation part. In the literature review, the COMSOL Multiphysics modeling tool and modeling process for paper drying will be introduced. In addition, the mathematical model which is used in the COMSOL Multiphysics modeling tool will be introduced briefly. In the simulation part, the new model and some comparison with earlier results will be introduced. Then the simulation results will be discussed.

2 Modeling of chemical engineering process

Process modeling is one of the key activities in process systems engineering. It is a significant activity in most major companies around the world, driven by such application areas as process optimization, design and control. (1, p. 13.)

2.1 The history of the modeling in process system engineering

As a distinct discipline, PSE is a child of the broader field of systems engineering as applied to processing operations. As such, its appearance as a recognized discipline dates back to the middle of the twentieth century. (1, p. 13.)

It was the industrial revolution which gave the impetus to systematic approaches for the analysis of processing and manufacturing operations. Sporadic examples of the use of systems engineering as a sub-discipline of industrial engineering in the nineteenth and twentieth centuries found application in many of the industrial processes developed in both Europe and the United States. In order to achieve this goal, there was a growing trend to reduce complex behavior to simple mathematical forms for easier process design, hence the use of mathematical models. (1, p. 13.)

Little existed in the area of process modeling aimed at reactor and separation systems. In the period from 1900 to the mid-1920s there was a fast growing body of literature on more detailed analysis of unit operations, which saw an increased reliance on mathematical modeling. Heat exchange, drying, evaporation, centrifugation, solids processing and separation technologies such as distillation were subject to the application of mass and energy balances for model development. (1, p. 14.)

After the end of the Second World War there was a growing interest in the application of systems engineering approaches to industrial processes, especially in the chemical industry. The mid-1950s saw many developments in the application of mathematical modeling to process engineering unit operations, especially for the understanding and prediction of the behavior of individual units. (1, p. 14.)

This interest in mathematical analysis coincided with the early developments and available growing of computers. This has been a major driving force in modeling ever

since. Some individuals, however, were more concerned with the overall process rather than the details of individual unit operations. (1, p. 15.)

Clearly, the vision of T.J. Williams was not met within the 1960s but tremendous strides were made in the area of process modeling and simulation. The seminal work on transport phenomena by Bird et al. in 1960 gave further impetus to the mathematical modeling of process systems through the use of fundamental principles of conservation of mass, energy and momentum. It has remained the pre-eminent book on this subject for over 40 years. (1, pp. 15-16.)

The same period saw the emergence of numerous digital computer simulators for both steady state and dynamic simulation. These were both industrially and academically developed tools. The development of mini-computers in the 1970s and the emergence of UNIX-based computers followed by the personal computer in the early 1980s gave a boost to the development of modeling and simulation tools. Accompanying the development of the process simulators was an attempt to provide computer aided modeling frameworks for the generation of process models based on the application of fundamental conservation principles related to mass, energy and momentum. (1, p. 16.)

What continues to be of concern is the lack of comprehensive and reliable tools for process modeling and the almost exclusive slant towards the petrochemical industries of most commercial simulation systems. The effective and efficient development of mathematical models for new and non-traditional processes still remains the biggest hurdle to the exploitation of those models in PSE. (1, p. 16.)

2.2 Fundamental principles

Mathematical models play a vital role in PSE. Nearly every area of application is undergirded by some form of mathematical representation of the system behavior. The form and veracity of such models is a key issue in their use. Over the last 50 years, there has been a widespread use of models for predicting both steady state and dynamic behavior of processes. This was principally in the chemical process industries but, recently, these techniques have been applied into other areas such as

minerals, pharmaceuticals and bio-products. In most cases these have been through the application of process simulation cooperating embedded models. (1, p. 17.)

2.2.1 Conservation principles

The underlying principles on which all process modeling takes place are based on thermodynamic concepts. Those thermodynamic concepts arise due to our current understanding about the nature of matter, confirmed by experiment and observation. In particular, the fundamental laws of physics provide us with a framework to describe the behavior of systems through a consideration of the mass, energy and momentum of the system in 3D space. We have to consider the fourth dimension of time where we are also interested in the time varying behavior of the system. (1, p. 42.)

In many applications of the conservation principles for mass, energy and momentum there will be cases where mass, energy or momentum will be transferred into or out of our balance volumes. This is especially the case where we deal with interacting phases involving mass or energy. Here, there are driving forces at work which can transfer material and energy between the phases. These driving forces are generally in terms of the intensive properties of the system. They include concentration, temperature and pressure differentials but can be extended to electrical potentials and other driving forces such as chemical potential.

Mass transfer involves a driving force in terms of chemical potential or equivalent intensive property such as concentration or partial pressure. Heat transfer takes place through the three principal mechanisms: conduction, radiation and convection. Each mechanism can be represented by specific forms of constitutive equations. (1, pp. 65-69.)

When heat is transferred from one body to another separated in space, then the key mechanism is radiative heat transfer. This is a common mechanism in high temperature process operations. Radiation occurs from all bodies and depends on the absolute temperature of the body and its surface properties. Convective heat transfer occurs as a result of the transfer of energy between a moving gas or liquid phase and a solid phase. The mechanisms can be divided into natural convection and

forced convection processes. In the first case, the fluid movement is induced by density differences created by temperature gradients. In the second case, the fluid movement is a result of mechanical motion induced by pumping action or driven by pressure differences. (1, pp. 69-70.)

Thermodynamic properties are absolutely essential to process systems modeling. In fact, they form the backbone of most successful simulations of process systems. Nearly all process based simulation systems have extensive physical properties packages attached to them. (1, p. 72.)

2.2.2 Constitutive relations

Constitutive relations are usually algebraic equations of mixed origin. The underlying basic thermodynamic, kinetic, control and design knowledge is formulated and added to the conservation balances as constitutive equations. This is because when we write conservation balances for mass, energy and momentum, there will be terms in the equations which will require definition or calculation. These requirements give rise to a range of constitutive equations which are specific to the problem.

Constitutive equations describe five classes of relations in a model:

- Transfer rates: mass transfer, heat/energy transfer;
- Reaction rate expressions;
- Property relations: thermodynamical constraints and relations, such as the dependence of thermodynamical properties on the thermodynamical state variables of temperature, pressure and composition. There are also equilibrium relations and equations of state;
- Balance volume relations: relationships between the defined mass and energy balance regions;
- Equipment and control constraints. (1, p. 65.)

2.3 Advanced process modeling and model analysis

The analysis of process system models leads to mathematical problems of various types. It is convenient and useful to formulate these mathematical problems in a formal way specifying the inputs to the problem, the desired output or question to be solved and indicate the procedure or method of solution. Such a formal problem

description can also be useful when we want to analyze the computational needs of a mathematical problem or one of its solution methods. (1, p. 251.)

Process modeling has found great utility in the design, control and optimization of process systems, and more recently, in the general area of risk assessment. In carrying out the necessary simulation studies, most process engineers make use of canned models offered in commercial simulation packages such as Aspen Plus (2), Aspen Dynamics or HYSYS to generate solutions to process engineering problems. Sometimes, customization of existing models must be developed.

The improvement and increasing importance of computational fluid dynamics (CFD) packages have provided a computer based modeling approach at the most complex end of the modeling spectrum, whilst general process model building tools still remain largely an academic curiosity. The CFD tools are extremely important for resolving complex fluid flow, heat and mass transfer problems in process vessels or in large-scale environmental systems. Their utility in these areas will inevitably be coupled with standard flowsheeting tools to span the complete spectrum of process modeling.

The key users of process modeling tools are the process industries. When we consider modeling in the process industries, there are a small number of very mature areas and a huge number of potential users. The petroleum and petrochemical industries have dominated the development of flowsheeting and modeling tools. The uptake of these tools and their widespread use has often been hampered by the difficulty of using the canned models in particular applications. The lack of tools to tackle process modeling at a level higher than the equation systems, where enormous amount of time, effort and money are expended, has often been an excuse for not taking up process model based applications.(1, pp. 472-473.)

3 Modeling software

Modeling software are used in a wide variety of industries. Simulation software is based on the process of modeling a real phenomenon with a set of mathematical formulas.

3.1 Aspen

Aspen Plus is a comprehensive chemical process modeling system, used by the world's leading chemical and specialty chemical organizations, and related industries to design and improve their process plants. Aspen Plus provides the widest array of tools to construct and optimize process models including best-in-class physical properties, ability to handle solid, liquid, and gas processes, and advanced electrolytes and equation oriented modeling mode. (2.)

Aspen Plus provides the widest array of tools to construct and optimize process models including best-in-class physical properties, ability to handle solid, liquid, and gas processes, advanced electrolytes and equation oriented (E/O) modeling mode. Aspen Plus boasts the world's most extensive property database and handles solid, fluid and gas phase processes - making it the best choice for chemicals, polymers, specialty chemicals, pharmaceuticals and biotech, biofuels, power, carbon capture, minerals, metals and mining. (2.)

Aspen Plus includes options to simulate polymer processes, batch distillation columns, and rate limited columns. Aspen Custom Modeler can be written additional unit operation models and use them inside Aspen Plus. Aspen Plus Dynamics can be used to evaluate process safety and operability, evaluate control strategies, or optimize grade and rate transitions. Aspen Plus can immediately be seen the economic impact of design changes, opportunities for energy savings can be identified, greenhouse gas emissions evaluated, and simulation and plant data side-by-side viewed. (2.)

Aspen Properties provides state-of-the-art physical property methods, models, algorithms, and data. Engineers and chemists can easily perform calculations based on rigorous, proven thermophysical property models and data. This information can then be captured and deployed. Aspen Properties directly accesses the National Institute of Standards and Technology (NIST) database that includes experimental data for over 24,000 pure components and 30,000 binary pairs. Aspen Properties also features built-in parameter estimation and data regression capabilities, even for non-idea chemicals, electrolytes, and solids. (2.)

Aspen Property models can be accessed through the Aspen Properties Add-In for Microsoft Excel. Powerful tools for: thermophysical and transport property estimation, phase-equilibrium calculations, and solubility modeling can be accessed from experimental data. The Aspen Pure Component Database, or the NIST Source Database and locate components can be searched based on their name, formula, or Chemical Abstract Service (CAS) registry number. (2.)

Aspen HYSYS is a comprehensive process modeling system used by world's leading oil & gas producers, refineries and engineering companies to optimize process design and operations. The process simulation capabilities of *Aspen HYSYS* enable engineers to rapidly evaluate the safest and most profitable designs through quick creation of interactive models for "what-if" studies and sensitivity analysis. These models can be leveraged throughout the plant life cycle—from conceptual to detailed designs, performance rating, and optimization—significantly reducing engineering costs and enabling better operating decisions. (3.)

The best modeling environment for the energy industry is now easier to use than ever before. Energy analysis and integrated heat exchanger modeling experienced the activated economics to optimize in minutes and realize more value. Aspen HYSYS provides industry specific capabilities that enable process engineers to solve the most pressing problems across the energy industry. Aspen HYSYS seamlessly enables dynamics, refining modeling, upstream design, and acid gas cleaning all with same easy to use interface. (3.)

Aspen HYSYS is an easy to use process modeling environment that enables optimization of conceptual design and operations. Aspen HYSYS has a broad array of features and functionalities that address the process engineering challenges of the energy industry. Aspen HYSYS can immediately be seen the economic impact of design changes, opportunities for energy savings can be identified, greenhouse gases tracked, and simulation and plant data side-by-side viewed. (3.)

Now dynamic simulation is just as accessible as steady state. Existing HYSYS models can be easily converted to run in dynamic mode, a rich set of control functionality can be experienced, and a comprehensive list of unit operations can be accessed. Aspen Simulation Workbooks integrates with other aspenONE Engineering software

to serve every stage of the process engineering lifecycle, including Aspen Plus, HYSYS, the EDR suite, Aspen Custom Modeler, and the Economics suite. (3.)

3.2 COMSOL Multiphysics

Since it is a multiphysics world, simulation tool must be multiphysics capable in order to correctly capture the important aspects of design. The COMSOL Multiphysics approach starts with first principles like transport phenomena, electromagnetic field theory, and solid mechanics as the basic fibers of the software. Then, in an elegant and flexible user interface, these fibers can be weaved together in a self-consistent way to solve particular simulation needs. (4.)

COMSOL Multiphysics is an interactive environment for modeling and solving all kinds of scientific and engineering problems. The software provides an integrated desktop environment with a Model Builder where you get full overview of the model and access to all functionality. With COMSOL Multiphysics conventional models for one type of physics can be extended into multiphysics models that solve coupled physics phenomena—and do so simultaneously. Accessing this power does not require an in-depth knowledge of mathematics or numerical analysis. (4.)

COMSOL Multiphysics delivers the ideal tool to build simulations that accurately replicate the important characteristics of designs. Its unparalleled ability to include all relevant physical effects that exist in the real world is known as multiphysics. (4.)

It would be ideal, then, to have a simulation environment that included the possibility to add any physical effect to model. That is what COMSOL is all about. It is a flexible platform that allows users to model all relevant physical aspects of their designs. Expert users can go deeper and use their knowledge to develop customized solutions, applicable to their unique circumstances. With this kind of all-inclusive modeling environment, COMSOL gives the confidence to build the model with real-world precision. (5, p. 6.)

Certain characteristics of COMSOL become apparent with use. Compatibility stands out among these. COMSOL requires that every type of simulation included in the package has the ability to be combined with any other. This strict requirement mirrors what happens in the real world. For instance in nature electricity is always

accompanied by some thermal effect; the two are fully compatible. Enforcing compatibility guarantees consistent multiphysics models and the knowledge that we never have to worry about creating a disconnected model again. (5, p. 6.)

Another noticeable trait of the COMSOL platform is adaptability. As modeling needs change, so does the software. If we find ourselves in need of including another physical effect, we can just add it. If one of the inputs to our model requires a formula, we can just enter it. Using tools like parameterized geometry, interactive meshing and custom solver sequences, we can quickly adapt to the ebbs and flows of our requirements. (5, p. 6.)

The flexible nature of the COMSOL environment facilitates further analysis by making “what-if” cases easy to set up and run. We can take our simulation to the production level by optimizing any aspect of our model. Parameter sweeps and target functions can be executed directly in the user interface. From start to finish, COMSOL is a complete problem-solving tool. (5, p. 6.)

Using these physics interfaces, we can perform various types of studies including:

- Stationary and time-dependent (transient) studies
- Linear and nonlinear studies
- Eigenfrequency, modal, and frequency response studies

When solving the models, COMSOL Multiphysics uses the proven finite element method (FEM). The software runs the finite element analysis together with adaptive meshing (if selected) and error control using a variety of numerical solvers. COMSOL Multiphysics creates sequences to record all steps that create the geometry, mesh, studies and solver settings, and visualization and results presentation. It is therefore easy to parameterize any part of the model: Simply change a node in the model tree and re-run the sequences. The program remembers and reapplies all other information and data in the model.

Partial differential equations (PDEs) form the basis for the laws of science and provide the foundation for modeling a wide range of scientific and engineering phenomena. We can use COMSOL Multiphysics in many application areas, for example:

- Acoustics
- Bioscience
- Chemical reactions
- Diffusion
- Electrochemistry
- Electromagnetics
- Fluid dynamics
- Fuel cells and electrochemistry
- Geophysics
- Heat transfer
- Microelectromechanical systems (MEMS)
- Microfluidics
- Microwave engineering
- Optics
- Photonics
- Plasma physics
- Porous media flow
- Quantum mechanics
- Radio-frequency components
- Semiconductor devices
- Structural mechanics
- Transport phenomena
- Wave propagation

Many real-world applications involve simultaneous couplings in a system of PDEs—multiphysics. For instance, the electric resistance of a conductor often varies with temperature, and a model of a conductor carrying current should include resistive-heating effects. The Multiphysics Modeling section discusses multiphysics modeling techniques. Many predefined multiphysics interfaces provide easy-to-use entry points for common multiphysics applications.

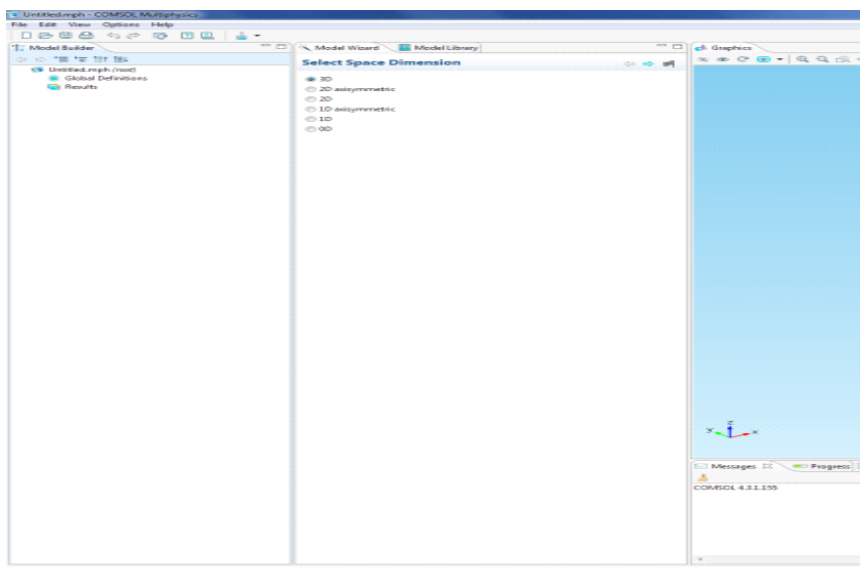
In its base configuration, COMSOL Multiphysics offers modeling and analysis power for many application areas. For several of the key application areas there are also optional modules. These application-specific modules use terminology and solution methods specific to the particular discipline, which simplifies creating and analyzing models.

The Transport of Diluted Species Interface provides a predefined modeling environment for studying the evolution of chemical species transported by diffusion and convection. The interface assumes that all species present are dilute; that is, that their concentration is small compared to a solvent fluid or solid. As a rule of thumb, a mixture containing several species can be considered dilute when the concentration of the solvent is more than 90 mol%. Due to the dilution, mixture properties such as density and viscosity can be assumed to correspond to those of the solvent. (5.)

Fick's law governs the diffusion of the solutes dilute mixtures or solutions, while the phenomenon of ionic migration is sometimes referred to as electrokinetic flow. The Transport of Diluted Species physics interface supports the simulation of chemical species transport by convection, diffusion, and migration in 1D, 2D, and 3D as well as for axisymmetric models in 1D and 2D. (5.)

3.3 The COMSOL desktop environment

The Desktop on the previous pages is what you see when you first start COMSOL. The COMSOL Desktop provides a complete and integrated environment for physics modeling and simulation. It can be customized according to needs. The Desktop windows can be resized, moved, docked and detached. Any changes to the layout will be saved when the session is closed and used again the next time when COMSOL is opened. As you build your model, additional windows and widgets will be added. (5.)



In Figure 1 is shown the main window for entering all of the specifications of the model, the dimensions of the geometry, the properties of the materials, the boundary conditions and initial conditions, and any other information that the solver will need to carry out the simulation.

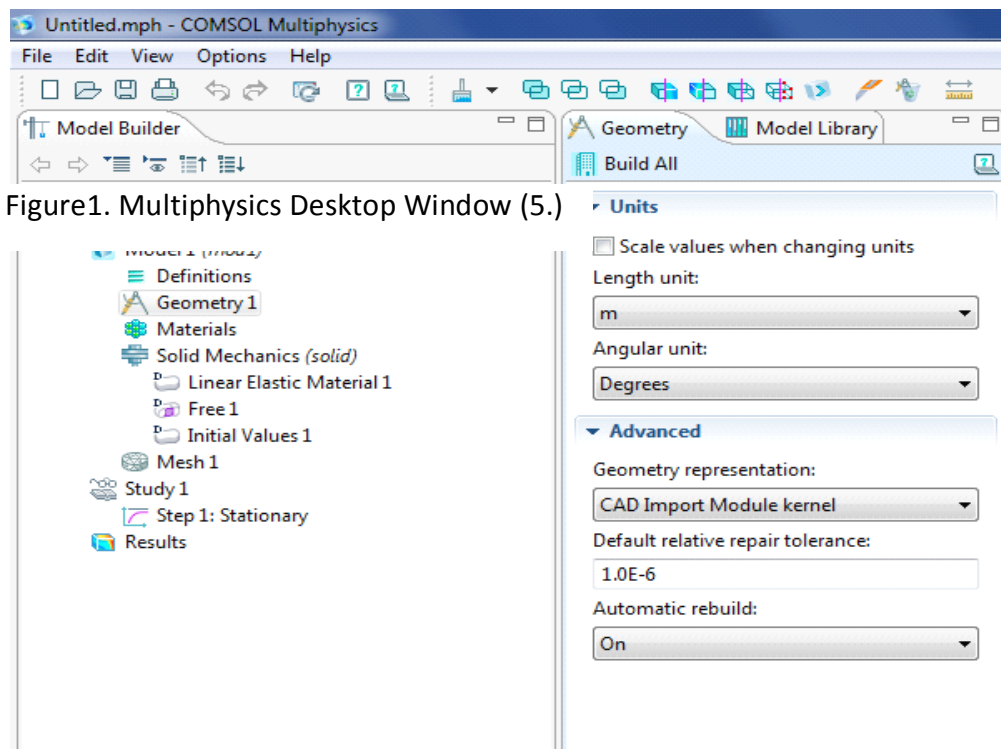


Figure1. Multiphysics Desktop Window (5.)

Figure 2. Model Builder Window (5.)

The Model Builder is the tool where the model is defined: how to solve it, the analysis of results, and the reports. It is done by building a Model Tree. The tree is built by starting with a default Model Tree, adding nodes, and editing the node settings. (5.)

Parameters are user-defined constant scalars that are usable throughout the Model Tree. It is important to know that the names of Parameters are case-sensitive. Parameters is defined in the Model Tree under Global Definitions. (5.)

Variables can be defined either in the Global Definitions node or in the Definitions subnode of any Model node. Naturally the choice of where to define the variable depends upon whether it needs to be global (i.e. usable throughout the Model Tree)

or locally defined with in a single one of the Model nodes. Like a Parameter Expression, a Variable Expression may contain numbers, parameters, built-in constants, and unary and binary operators. However, it may also contain Variables, like t , x , y , or z , functions with Variable Expressions as arguments, and dependent variables that solved for as well as their space and time derivatives. (5.)

The “scope” of a Parameter or Variable is a statement about where it may be used in an expression. As we have said, all Parameters are defined in the Global Definition node of the model tree. This means that they are global in scope and can be used throughout the Model Tree. (5.)

A Variable may also be defined in the Global Definitions node and have global scope, but they are subject to limitations other than their scope. For example, Variables may not be used in Geometry, Mesh, or Study nodes (with the one exception that a Variable may be used in an expression that determines when the simulation should stop). (5.)

A Variable that is defined, instead, in the Definitions subnode of a Model node has local scope and is intended for use in that particular Model (but, again, not in Geometry or Mesh nodes). They may be used, for example, to specify material properties in the Materials subnode or to specify boundary conditions or interactions. It is sometimes valuable to limit the scope of the variable to only a certain part of the geometry, such as certain boundaries. For that purpose, provisions are made in the Settings for a Variable definition to apply the definition either to the entire geometry of the Model, or only to certain Domains, Boundaries, Edges, or Points. (5.)

COMSOL comes with many built-in constants, variables and functions. They have reserved names that can not be redefined by the user. If a reserved name is used for a user-defined variable, parameter, or function, the text where the name is entered will turn orange (a warning) or red (an error) . (5.)

Some important examples are:

- Mathematical constants such as the imaginary unit i or j

- Physical constants such as g const (acceleration of gravity), c const(speed of light), or R const (universal gas constant)
- The time variable t
- First and second order derivatives of the Dependent variables (the solution) whose names are derived from the spatial coordinate names and Dependent variable names (which are user-defined variables)
- Mathematical functions such as cos, sin, exp, log, log10, and sqrt. (5, pp. 7-17.)

Animating a solution to a physical problem can be very helpful in understanding the underlying physical phenomena. Sometimes such animations can give rise to new questions and inspire creativity. (6.)

4 Mathematics model

A mathematical model is a description of a system using mathematical concepts and language. The process of developing a mathematical model is termed mathematical modeling. Mathematical models are used not only in the natural sciences and engineering disciplines, but also in the social sciences. A model may help to explain a system and to study the effects of different components, and to make predictions about behaviour.

4.1 Basic equations of mass and heat transfer

The default node attributed to the Transport of Diluted Species interface assumes chemical species transport through diffusion and convection (a button to activate migration is readily available) and implements the mass balance equation:

$$\frac{\partial c}{\partial t} + u \cdot \nabla c = \nabla \cdot (D \nabla c) + R \quad (1)$$

Equation (1) includes these quantities (with the SI unit in parentheses):

C is the concentration of the species (mol/m³)

D denotes the diffusion coefficient (m²/s)

R is a reaction rate expression for the species (mol/(m³·s))

u is the velocity vector (m/s)

There are two different ways to present a mass balance where chemical species transport occurs through diffusion and convection. These are the non-conservative and conservative formulations of the convective term:

non-conservative:

	$\frac{\partial e}{\partial t} + u \cdot \nabla c = \nabla \cdot (D \nabla c) + R$	(2)
--	--	-----

conservative:

$$\frac{\partial e}{\partial t} + \nabla \cdot (cu) = \nabla \cdot (D \nabla c) + R \quad (3)$$

And each is treated slightly differently by the solver algorithms. In these equations D is the diffusion coefficient (SI unit: m²/s), R is a production or consumption rate expression (SI unit: mol/(m³·s)), and u is the solvent velocity field (SI unit: m/s). The diffusion process can be anisotropic, in which case D is a tensor.

If the conservative formulation is expanded using the chain rule, then one of the terms from the convection part, $c \nabla \cdot u$, would equal zero for an incompressible fluid and would result in the non-conservative formulation above. This is in fact the default formulation in the Transport of Diluted Species interface and ensures that nonphysical source terms cannot come from the solution of a flow field.

4.2 Computational fluid dynamics-CFD

Computational fluid dynamics, usually abbreviated as CFD, is a branch of fluid mechanics that uses numerical methods and algorithms to solve and analyze problems that involve fluid flows. Computers are used to perform the calculations required to simulate the interaction of liquids and gases with surfaces defined by boundary conditions. With high-speed supercomputers, better solutions can be achieved. Ongoing research yields software that improves the accuracy and speed of complex simulation scenarios such as transonic or turbulent flows. (7.)

In all of these approaches the same basic procedure is followed.

- During preprocessing
 - The geometry (physical bounds) of the problem is defined.
 - The volume occupied by the fluid is divided into discrete cells (the mesh). The mesh may be uniform or non-uniform.
 - The physical modeling is defined – for example, the equations of motions + enthalpy + radiation + species conservation
 - Boundary conditions are defined. This involves specifying the fluid behavior and properties at the boundaries of the problem. For transient problems, the initial conditions are also defined.
- The simulation is started and the equations are solved iteratively as a steady-state or transient.
- Finally a postprocessor is used for the analysis and visualization of the resulting solution. (7.)

Discretization methods

The stability of the chosen discretization is generally established numerically rather than that of analytically as with simple linear problems. Special care must also be taken to ensure that the discretization handles discontinuous solutions gracefully. The Euler equations and Navier–Stokes equations both admit shocks, and contact surfaces. (7.)

Some of the discretization methods being used are:

Finite volume method

the finite volume method (FVM) is a common approach used in CFD codes, as it has an advantage in memory usage and solution speed, especially for large problems, high Reynolds number turbulent flows, and source term dominated flows (like combustion) (7).

In the finite volume method, the governing equations partial differential equations (typically the Navier-Stokes equations, the mass and energy conservation equations, and the turbulence equations) are recast in a conservative form, and then solved over discrete control volumes. This discretization guarantees the conservation of fluxes through a particular control volume. (7.)

Finite element method

The finite element method (FEM) is used in structural analysis of solids, but is also applicable to fluids. However, the FEM formulation requires special care to ensure a conservative solution. The FEM formulation has been adapted for use with fluid dynamics governing equations. Although FEM must be carefully formulated to be conservative, it is much more stable than the finite volume approach. However, FEM can require more memory and has slower solution times than the FVM. (7.)

Finite difference method

The finite difference method (FDM) has historical importance and is simple to program. It is currently only used in few specialized codes, which handle complex geometry with high accuracy and efficiency by using embedded boundaries or overlapping grids (with the solution interpolated across each grid). (7.)

4.3 Finite element method--FEM

In mathematics, finite element method (FEM) is a numerical technique for finding approximate solutions to boundary value problems. It uses variational methods (the Calculus of variations) to minimize an error function and produce a stable solution. Analogous to the idea that connecting many tiny straight lines can approximate a larger circle, FEM encompasses all the methods for connecting many simple element equations over many small subdomains, named finite elements, to approximate a more complex equation over a larger domain. (8.)

4.3.1 General principles

A feature of FEM is that it is numerically stable, meaning that errors in the input and intermediate calculations do not accumulate and cause the resulting output to be meaningless. In the first step above, the element equations are simple equations that locally approximate the original complex equations to be studied, where the original equations are often partial differential equations (PDE). To explain the approximation in this process, FEM is commonly introduced as a special case of Galerkin method. The process, in mathematics language, is to construct an integral of the inner product of the residual and the weight functions and set the integral to zero. In simple terms, it is a procedure that minimizes the error of approximation by

fitting trial functions into the PDE. The residual is the error caused by the trial functions, and the weight functions are polynomial approximation functions that project the residual. (8.)

4.3.2 Application

Variety of specializations under the umbrella of the mechanical engineering discipline (such as aeronautical, biomechanical, and automotive industries) commonly uses integrated FEM in design and development of their products. Several modern FEM packages include specific components such as thermal, electromagnetic, fluid, and structural working environments. In a structural simulation, FEM helps tremendously in producing stiffness and strength visualizations and also in minimizing weight, materials, and costs. (8.)

FEM allows detailed visualization of where structures bend or twist, and indicates the distribution of stresses and displacements. FEM software provides a wide range of simulation options for controlling the complexity of both modeling and analysis of a system. Similarly, the desired level of accuracy required and associated computational time requirements can be managed simultaneously to address most engineering applications. FEM allows entire designs to be constructed, refined, and optimized before the design is manufactured. (8.)

This powerful design tool has significantly improved both the standard of engineering designs and the methodology of the design process in many industrial applications. The introduction of FEM has substantially decreased the time to take products from concept to the production line. It is primarily through improved initial prototype designs using FEM that testing and development have been accelerated. In summary, benefits of FEM include increased accuracy, enhanced design and better insight into critical design parameters, virtual prototyping, fewer hardware prototypes, a faster and less expensive design cycle, increased productivity, and increased revenue. (8.)

4.4 Distributed parameter model

In most cases, heat transfer is inherently a distributed process. This has been a very common application area spanning 1D, 2D and 3D modeling. Applications range from

double-pipe heat exchangers of one spatial variable through to irregular shaped non-homogeneous 3D bodies with complex boundary conditions. (1, p. 174.)

Partial differential equations (PDEs) occur in many process engineering applications from fluid flow problems to heat transfer. Generally, most problems lead to parabolic equations which are time independent and hence represent unsteady-state processes. In contrast, steady-state problems lead to elliptic PDEs. (1, p. 191.)

Many numerical techniques have been developed to solve PDEs. The most widely used are still the finite difference methods, which are generally much simpler to set up compared with other available methods. However, in the last 20 years, and especially the last 10 years the finite element method has been used to solve many problems with irregular shaped boundaries as well as a diverse range of problems. In chemical reactor analysis, the orthogonal collection technique has also been extensively used because of reasons of accuracy and efficiency. Another popular method often used is the method of lines, which converts a PDE to a set of ODEs subsequently using efficient ODE codes to solve the sets of equations. The choice between methods for a particular problem is not always an easy one. It is often a matter of experimentation, since many factors have to be considered. These include the complexity of the problem, ease of setting up the solution method, accuracy required, stability problems and computational effort. (1, p. 191.)

5 Application area: paper manufacture and coated paper drying

In this paper, we will talk about the applications of Models in the areas of paper manufacture and paper drying. To understand the modeling in papermaking processes and paper drying more easily.

5.1 Modeling in the papermaking processes

Customer needs and global competitions have made specialized and tailor-made products an essential part of the economic success in the paper industry. As a result more paper grades are manufactured nowadays than earlier. In some paper machines this has increased the number of grade changes. (9) A grade change is a

product quality change on a paper machine. Today's high quality papers require a highly technical and accurate manufacturing process. So it has to be monitored and controlled continuously in order to ensure that the qualities of paper products stay within their specifications.

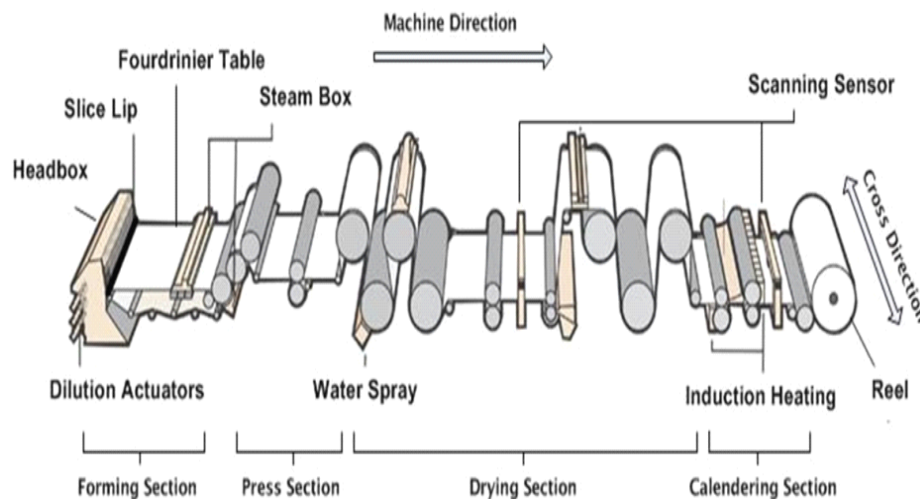


Figure3. The configuration of a Fourdrinier-type paper machine(11)

In history, there are so many approaches to improve the grade change methods, so many models were applied in papermaking processes. For example, MPC perhaps which is the most straightforward method to apply optimizing controls to a grade change. In addition to that Murphy and Chen (2000) used a combination first-order plus delay models including total head coordination model for the headbox. McQuillin and Huizinga (1994) reported the use of a model predictive control. Kuusisto et al. (2002) used second order transfer function models (ARX) in the MPC control.

The improvement in the duration of a grade change could be achieved by calculating the target values of the manipulated variable more accurately than in the existing approaches. So a method, hybrid modeling is proposed.

In this part, we talk about the hybrid modeling in papermaking processes mainly to lead the reader to understand the importance and the generalized application of

modeling in this area.

5.2 Hybrid Modeling for a Paper Machine Grade Change

Hybrid modeling is a combination of empirical and physical modeling. It is one way to exploit a priority and experimental information in a modeling context.

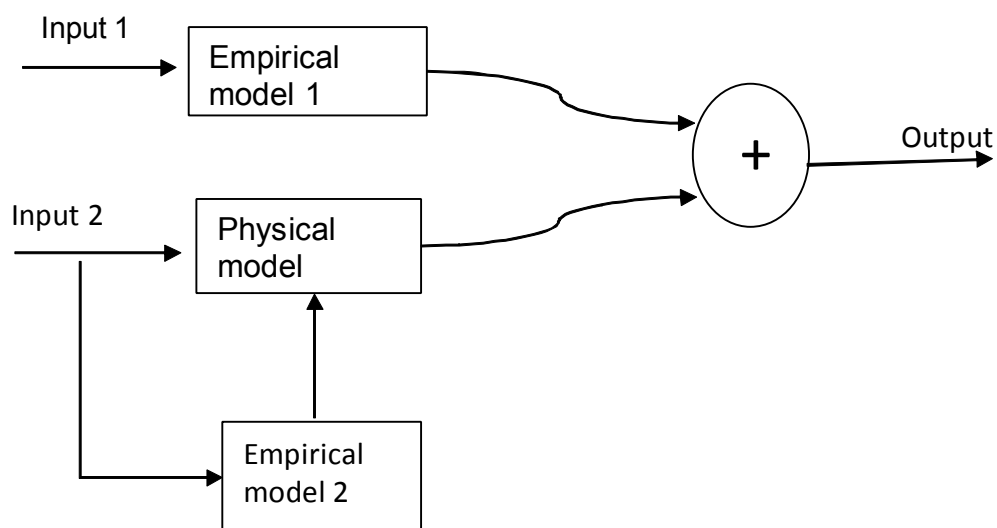


Figure4. Structure of the proposed hybrid model

A hybrid modeling structure that combines simple physical models with PLS in parallel and another empirical model that is used to adjust parameters of the physical model is proposed to complicated modeling problems of grade change on a paper Machine.

The set of models can be chosen according to the structure of the target paper machine. It is the task of the optimization to choose and adjust the parameters of the physical models. It brings in a new way to implement priority information in the hybrid modeling scheme.

5.2.1 Hybrid models for drying of paper

A good model for drying of web is a key element to a successful grade change because it is assumed to be the most significant factor of performance improvement.

The hybrid model of drying of paper consists of a physical model of drying section

and an empirical model. The empirical model corrects the modeling error of the physical model. The physical model uses the information of the drying section and the empirical model uses the data from the raw materials of the stock flows. The target values of head box settings (slice, jet-to-wire) and lineal pressures of the press section are not usually known before grade change. However, it is possible to include them in the static model for the evaluation of possible grade change options. (9.)

5.2.2 Hybrid model for basis weight

The steady state value of the basis weight can be considered to depend mostly on the machine speed and thick stock flow. Basis weight depends also on shrinkage and elongation of the web due to drying and winding stress. However, several variables are included in the empirical model.(9.)

In this work a very simple physical basis weight model was used to predict the new basis weight after the grade change. The same model can be used also to predict target values for machine speed and thick stock flow.(9.)

The empirical model is used to correct the gain of the physical model. The empirical model includes for example variables from the proportioning, refining, head box (slice, jet-to-wire ratio) and steam pressures. The steam pressures are expected to take into account the shrinkage effects into the model.(9.)

5.3 Modeling in economic optimization

The MPC control is always used in the economic optimization in papermaking processes. Paper-making is a very energy-intensive industrial activity. UK 2008 figures:

Paper Type	Energy Consumed
Packaging board	2 – 3 MWhr/t paper made
Newsprint	3 – 4 MWhr/t
Tissue	5 – 7 MWhr/t
Fine Papers	4 – 8 MWhr/t
Specialty papers	Up to 20 MWhr/t
UK Average	4 MWhr/t

Figure 5 Energy Consumption of making different types of Paper (12)

Present day pulp & paper industry processes were designed when energy was cheap and plentiful:

- About 70 paper machines are still operated in the UK (>200 50 years ago)
- Each machine costs £10s of millions each; not easy to change technology fast

The rising cost of energy has shut more than 10 UK paper mills in the last three years; and the same is elsewhere in Europe. So to optimize and better control energy use in paper making is extremely urgent. The MPD can solve this problem effectively.(10)

Multivariable Model predictive control (MPC) as a popular technology has been a prominent part of APC ever since supervisory computers first brought the necessary computational capabilities to control systems in the 1980s.(10)

A successful approach to reducing energy consumption in paper making needs to make coordinated, coherent use of such variables as:

- Refining of stock
- Headbox properties
- Drainage, including:
 - Rate of use of drainage aids (often presently just dosed on a wt/wt basis)
 - Vacuums (remain unused for any closed loop control purposes at present)
 - Press parameters (also largely unused in real time)
 - Optimization of the dryer, including pressures, differential pressures and condensate recovery rates (most of these are presently unused for control).

Advanced Process Control has tools that do these things in real time.

5.4 Coated Paper Drying

Drying of coated paper is a complex process that includes the three mechanisms of heat transfer (conduction, convection, and radiation) coupled with water (liquid, vapor and bound), air, and binder mass transfer.

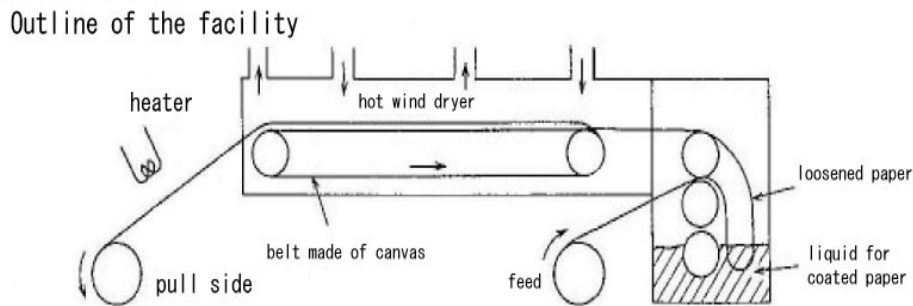


Figure 6. Equipment schematic diagram (11.)

During drying, liquid flows to the coating surface to feed evaporating water and toward the base stock driven by capillary pressure. At the evaporating surface, soluble binder such as starch will concentrate locally at a speed governed by the drying rate. In lieu of no other effects, binder deposition would occur regardless of the evaporation rate. However, a soluble binder will tend to restore concentration by means of mass diffusion of its molecules through the solvent. If the evaporation rate remains below the diffusion rate, no binder migration would be recorded. However, if evaporation rate surpasses diffusion rate, binder will concentrate on the surface. (11.)

5.4.1 Factors affecting the successful drying of coated papers

Drying is one part of the quality formation process of coated paper. During the past 20 years there have been tens of studies on how drying affects quality - especially the quality of offset papers. (10) There are a number of factors which will determine the likelihood of coated paper sticking together:

5.4.1.1 The type of coated paper

Paper may be gloss coated, dull-coated, machine-coated or cast-coated. To make a gloss-coated sheet, the matte-coated paper is supplementary processed by calendaring, a process where the paper is run through a stack of highly polished steel rollers which condenses and evens out surface inconsistencies. Dull-coated is made when a clay or chemical solution is added. When a clay solution is added to a base stock, the paper is considered matte-coated. Machine-coated is a sheet made

smooth by a blade running over it during the manufacturing process. The last, cast-coated, is a high-gloss coating used for the highest quality premium papers on one or both sides. (15.)

5.4.1.2 The method of drying

Three methods are commonly used for the drying of coated paper: IR drying (infrared radiation), air flotation drying and cylinder drying.

IR dryers

Gas infrared dryers have replaced electrical infrared dryers in coating drying solutions during the last decades. The disadvantage of gas IR dryers is poor energy economy.(15)

IR air combination dryer

Because the energy efficiency of IR dryers is much lower than that of air or cylinder dryers, efforts have been made to combine the advantages of both IR and air dryers. The resulting combined dryers have more blowing nozzles, which have helped to eliminate the weaknesses of IR dryers. But a continuing disadvantage is that paper which contains mechanical pulp (TMP, GW, and PGW) suffers from severe fiber rising when dried by a gas combination dryer.(15)

Air dryers

The air dryers used in coating machines can be divided into two categories: air flotation dryers and single-sided air impingement hoods. In an air flotation dryer, the web is supported on both sides by air jets or air cushions. Special flotation nozzle constructions have been developed to maintain good web stability and efficient heat transfer. (15)

Cylinder dryers

Cylinder dryers can be used only after the coating layer is immobilized and can withstand mechanical contact. Therefore, the cylinder section is normally the last drying phase of coating. In addition to its drying effect, the cylinder section pulls the paper web forward. (10.)

5.4.1.3 Drying speed

There will be alligatoring or mud cracking of coating during drying if coating is drying too fast to flow out. So we can reduce warm air supply, specify a medium drying speed coating. Or Anti-cracking lever is broken to solve these problems.

5.4.2 Some model researches in coated paper drying

Coated paper drying is a complex process and there are many factors to affect the quality of coated paper. So many types of models have been built to optimize the process and to improve the quality of coated paper, and many types of model applied in coated paper drying.

In an effort to improve coating qualities, researchers have attempted to correlate binder migration with the drying rate and its history. Despite the complexity of coating composition, pore structure, and coating–base-paper interaction, the mechanisms of drying and binder migration have been established. Capillarity-driven liquid flow, binder diffusion, and convection determine how binder distributes. Nowicki et al. used two-dimensional networks to simulate and analyze the pore-scale physics of a drying paper coating. Continuing in this line of investigation—with the aim of understanding liquid movement and binder migration in drying paper coatings—some researchers developed a three-dimensional pore-scale network model to examine broader ranges of drying rate and binder diffusivity than occur in industrial practice. (14.)

6 Paper drying models

In paper industry, drying simulation programs can be used in order to calculate new drying arch or to optimize paper quality through better moisture profile or adequate non-contact dryer location. Many models have been built in the area of Paper drying.

6.1 Model Formulation

The mass and energy conservation equations should account for the various boundary conditions resulting from the different drying methods that can be applied.

A proper model formulation should account individually for conservation of mass per species by taking into account all of its phases. The species of concern are given below.

- Water: gas, liquid, and bound
- Air: gas
- Particulate binder: solid
- Soluble binder: liquid and solid

A working model should provide temperature, moisture, binder concentration, and gas pressure distribution within the base stock and coating widths and along the machine direction. A correlation of the model results with experimental data might be used to determine the onset of mottle.(13)

6.2 Some models

There are so many models of coated paper drying now. Such as Farkas, Lampinen and Ojala Model, Heikkilae Model, Bernarda and Bruneau Model, Rajala and Karlsson Model, Nowicki Davis and Scriven Pan, Davis and Scriven Models etc.. The first four are macroscopic, one dimensional, and time dependent models, while the last two are microscopic two and three dimensional models, respectively. All models assume homogeneous properties, with constant intrinsic densities of the species. The models also assume that gravity and inertia forces are negligible. We will talk about some of these models in detail in this chapter.(12)

6.2.1 Farkas, Lampinen and Ojala Model

The authors (Farkas et al., 1991) developed a model to simulate drying of coated paper. The model accounts for binder migration by using a mass balance per species on a differential control volume. The energy equation is used to model temperature distribution along the paper thickness. Binder concentration, moisture content and temperature can be found as a function of time and in the direction of the paper thickness. (12)

6.2.2 Heikkilä Model

The Heikkilä (1993) model empirically accounts for drainage of liquid water into the base stock. It predicts the temperature and moisture distribution within the paper

and coating as a function of time and position. This model does not provide mass conservation equations for the individual species present, thus it cannot account for diffusion and migration of binder within the coating. Rewetting is modeled accounting for the differences in capillary pressure between the wet coating and the dry base stock. (12)

6.2.3 Bernarda and Bruneau Model

Bernarda and Bruneau's model (1995) accounts for the water, pigments, and binder transport with prediction of coating shrinkage not estimated by any other model. It uses a mass balance for an isothermal control volume within the coating. It does not account for the interactions between the coating and the base stock. Most of the transport mechanisms are empirically accounted and because no energy equation is developed, no prediction of temperature distribution is attempted.(12)

6.2.4 Rajala and Karlsson Model

Rajala and Karlson (1995) describe the efforts of VTT Energy in developing a model to simulate drying of coated paper without considering binder migration. The numerical results of the drying model are then correlated with coating defects, primarily mottle. The model accounts for the water mass balance and energy conservation equation. No binder migration is accounted in the model. After the temperature and moisture profiles are obtained, mottle is correlated with the operating parameters of the machine.(12)

6.2.5 Nowicki Davis and Scriven Pan, Davis and Scriven Models

In two different works, these authors describe a microscopic model to simulate moisture distribution and binder migration in drying of coated paper. In the first model, Nowicki et al., (1991 and 1993) develop a two dimensional microscopic model. The second model (Pan et al., 1995) is a three dimensional version of the previous one. Macroscopic behavior is inferred from the microscopic results. Moisture distribution and binder migration are accounted for in the coating only. (12)

6.3 Comparison of Drying Models for coated paper

	Farkas, Lampinen, and Ojala	Heikkilae	Bernarda & Bruneau	Rajala & Karlsson	Nowicki et al. and Pan
Country	Finland + Hungary	Finland	France	Finland	USA (Minnessota)
Scope	Macro	Macro	Macro	Macro	Micro
Include paper	Yes	Yes	No	Yes	No
Species mass bal.	Yes	No	Yes	No	Yes
Binder migration	Yes	No	Yes	No	Yes
Shrinkage	No	No	Yes	No	No
Rewetting	Yes	Yes	No	Empirical	No
Binder type	No	No	No	No	No
1D, transient energy eq.	Yes	Yes	No	Yes	No
Evaporation	Yes	Yes	Empirical	Yes	Yes
Conduction	Yes	Yes	No	Yes	No
Convection	No	No	No	No	No
Radiation	Exp. Absorpt. Coeff.	Linear	No	Constant	No
Mottle prediction	No	No	No	Yes	Yes
Validation results	Limited	Yes	Yes	Yes	Qualitative

Table1. Comparison of Drying Models for Coated Paper (12)

	Farkas et al.	Heikkilae	Bernarda & Bruneau	Rajala & Karlsson	Nowicki et al. and Pan et al.
Evaporation	Diffusion (Fick's Law)	Stephan's Law	Empirical	Diffusion	Diffusion
Vapor Flow	Diffusion (Fick's Law)	Stephan + Knudsen	Diffusion	Diffusion	Diffusion
Liquid Flow	Darcy's Law	Darcy's Law	Experimental	Darcy's Law	Stokes flow
Drainage	Darcy's Law	Lucas - Washburn	No	No	No
Binder migration	Diffusion	No	Diffusion	No	Diffusion

Table2. Comparison of Transport Mechanisms Used on Drying Models for Coated Paper. (12)

7 Experimental part

On the basis of the past experiment data, the model have been built by the COMSOL Multiphysics. We got the results of the simulation and compared them with the past results.

7.1 Model description

According to Darcy's law and Hagen-Poiseuille's law for liquid flows, the diffusion coefficient of the liquid water is obtained theoretically. The liquid flow affected by the surface tension and the gravity, the water vapor sorption/desorption by fibers, the diffusion of the water vapor and the phase changes are all taken into account in this model. With specification of initial and boundary conditions, distributions of water vapor concentration in void spaces, volume fraction of liquid water, distribution of water molecular content in fibers and temperature changes in paper web are obtained numerically. Effects of porosity of paper web on heat and mass transfer are analyzed.

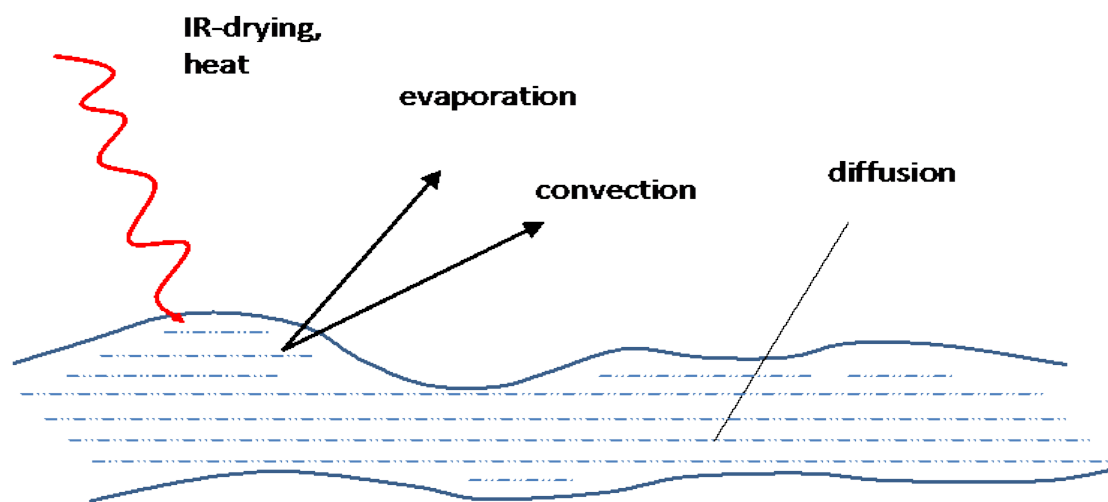


Figure6. Heat and mass transfer in paper web

As starting point we used Lampinen, Farkas model as starting point, we use the constant and conditions as in the Lampinen, Farkas model. However, we simplified their model, we just modeled the base paper in which there is only one component--water moving. In our model, finally, for some reasons, we just modeled the vapor diffusion phenomena successfully. So there is no capillary diffusion process and because we chose the base paper as our study target, there is no coating layer consequently no latex in our model.

But by simplifying the model with using this kind of tool, we have learned how to use it to model some basic physics and chemical phenomena. Of course, we achieved our purpose of comparing results of this model with more accurate model by Farkas,

Lampinen. Therefore, we got the conclusion that this kind of simplified model can even qualitatively be used to model drying.

7.2 Results and comparison with earlier results

In order to build the model with COMSOL Multiphysics modeling tool, firstly, we simulate a small piece from the vertical direction which is perpendicular to the web direction. We assume that there is no difference in any aspects in the web direction.

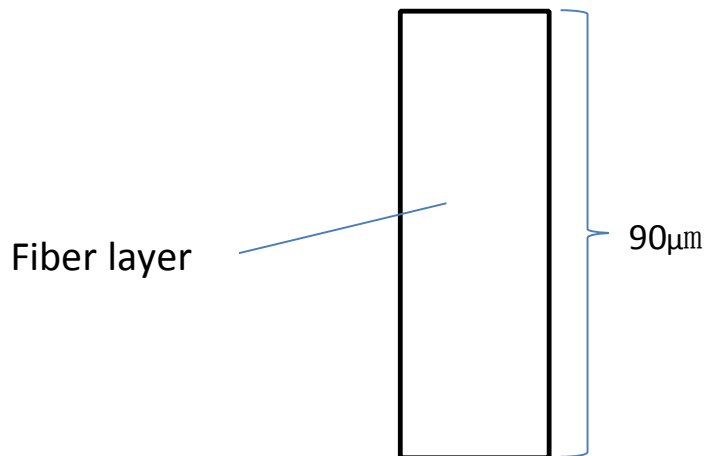


Figure 8. Geometry of the domain

The model we built is 1 dimensional, first we added Transport of Diluted Species (chds) and Heat Transfer (ht) physics and we selected the Time Dependent study type. The input data is shown in the following table:

Input data	value
$D_c, \text{m}^2/\text{s}$	2.7×10^{-5}
$C_0, \text{mol}/\text{m}^3$	1.3×10^3
$K_{c,c}, \text{m}/\text{s}$	1.0×10^{-3}
$C_{b,c}, \text{mol}/\text{m}^3$	2.3

Table3. Initial value of Transport of Diluted Species (chds)

$K, \text{W}/(\text{m}\cdot\text{k})$	0.05
$P, \text{Kg}/\text{m}^3$	670

Cp, J/(kg·K)	1400
T ₀ , K	310
h, W/(m ² ·k)	40
T _{ext} , K	333
Q, W/m ²	0.57 × 10 ⁹

Table4. Initial value of Heat Transfer (ht)

Formula for conversion between moisture and concentration:

$$m = c \cdot 0.018 [\text{kg/mol}] / (c \cdot 0.018 [\text{kg/mol}] + 670 [\text{kg/m}^3]) \cdot 100$$

The data were exported from the model then we depicted the following figures which give the comparison of our model with Lampinen, Farkas model. In our model it was demonstrated that the temperature increased sharply during the first 0.03 seconds. Consequently, the water diffused fast during that time. And the temperature was almost at the same level after that. The highest temperature was around 330K. However, in Lampinen, Farkas model, the temperature increased gradually and the temperature increase mainly focused on the first 0.25 seconds then it decreased. The highest temperature was 360K. The main reason maybe that the radiation heat transfer coefficient is constant in our model so that the temperature was almost at the same level.

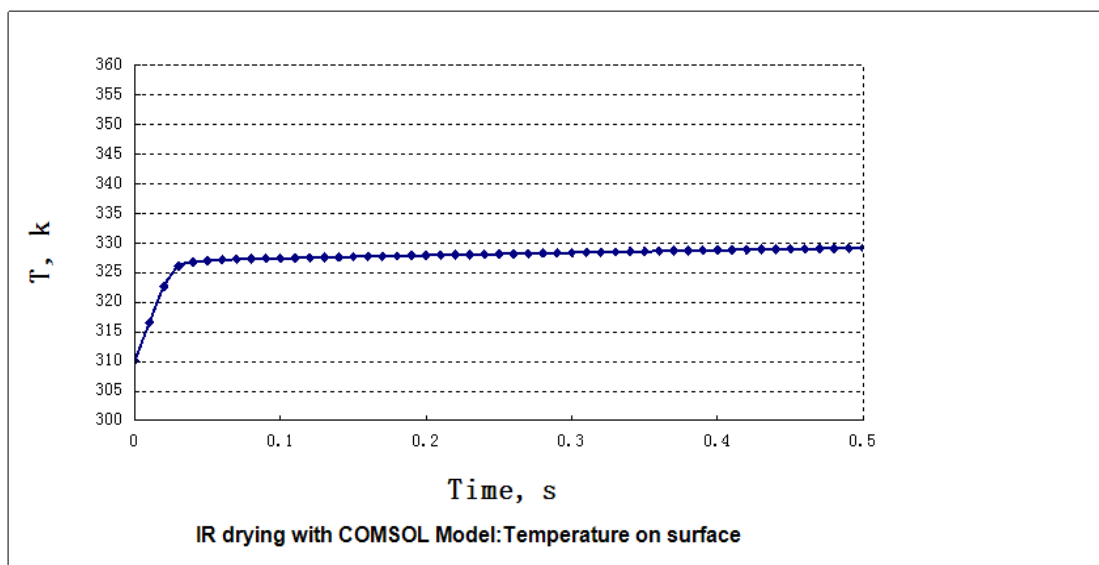


Figure 9. Temperature vs. Time (ir drying in our model: temperature on the surface)

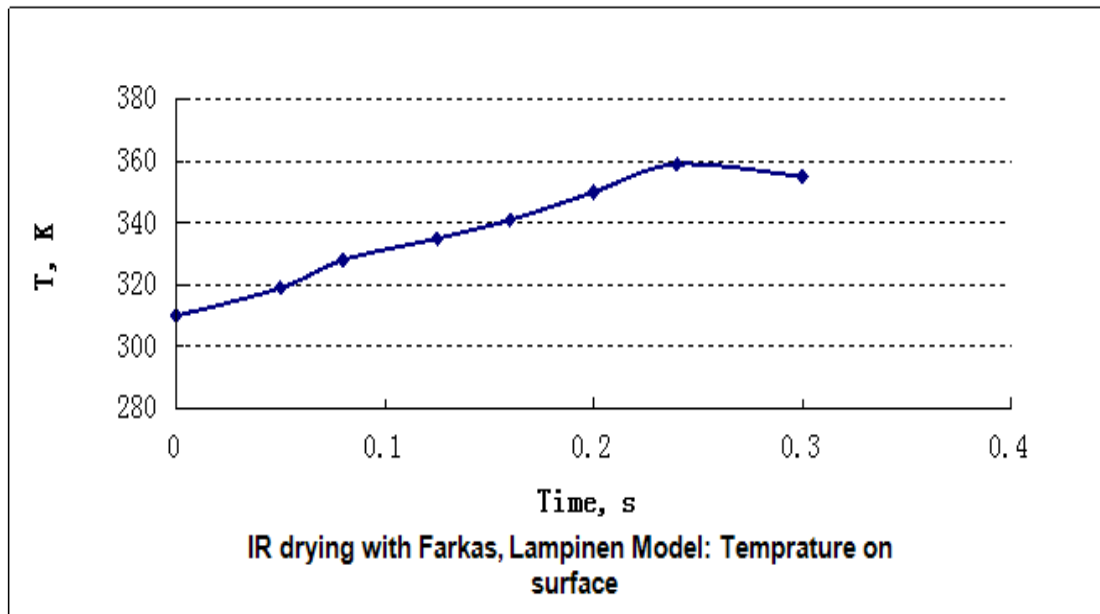


Figure 10. Temperature vs. Time (ir drying in Lampinen, Farkas model: temperature on the surface)

From the following figure, the trends during the first 0.4 second were almost same between our model and Lampinen, Farkas model. After that, in our model, the temperature raised sharply then reached the highest point 375K. The main reason for it maybe is that our model is too simple and we did not take the evaporation into account so that there was large difference between our model and Lampinen, Farkas model.

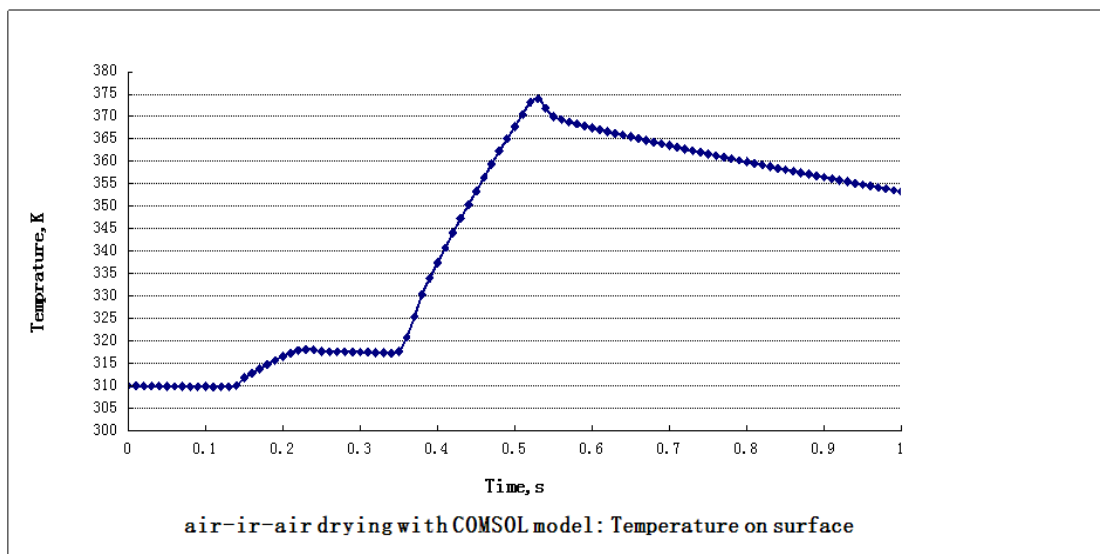


Figure 11. Temperature vs. Time (air-ir-air drying in our model: temperature on the surface)

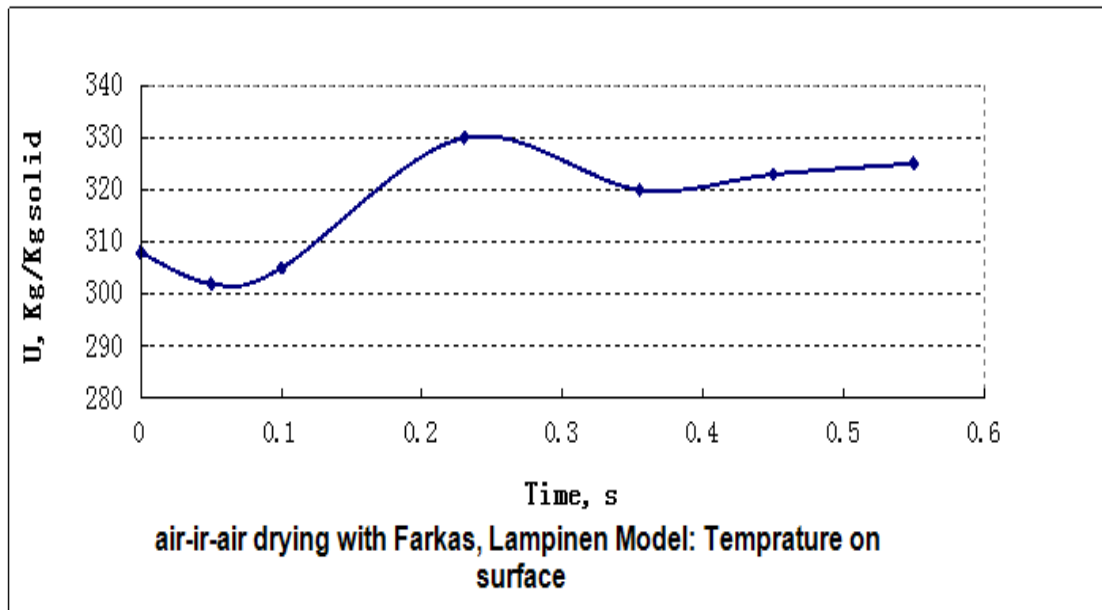


Figure 12. Temperature vs. Time (air-ir-air drying in Lampinen, Farkas model: temperature on the surface)

The moisture comparison was much different because our model was not very correct and did not take any phenomena into account. It was too simple.

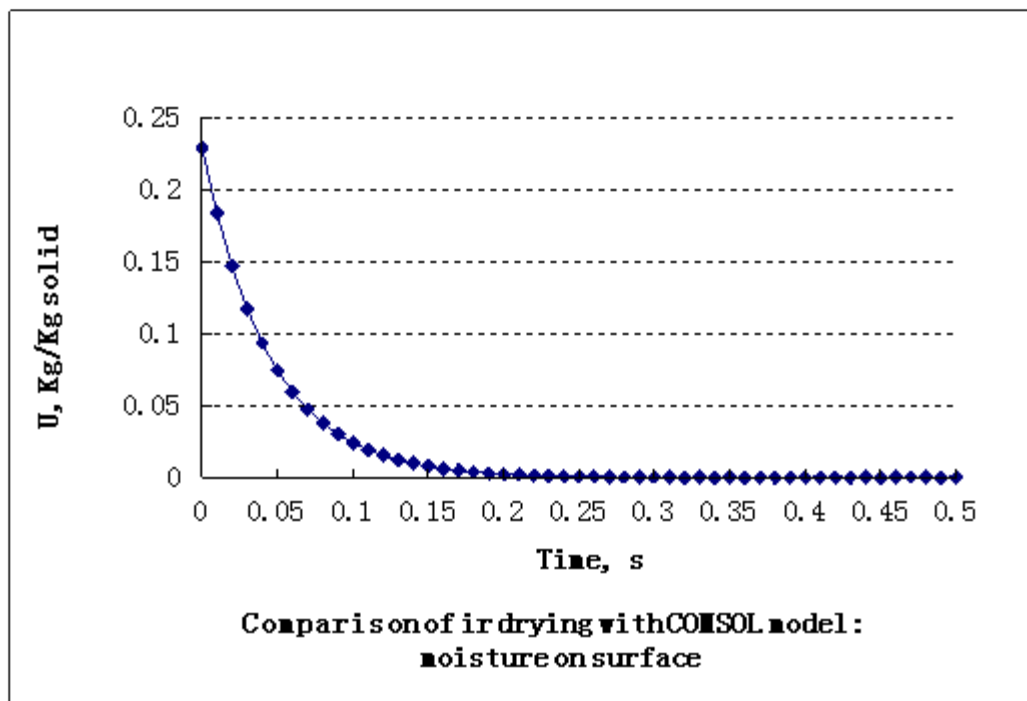


Figure 13. Moisture vs. Time (ir drying in our COMSOL model: moisture on the surface)

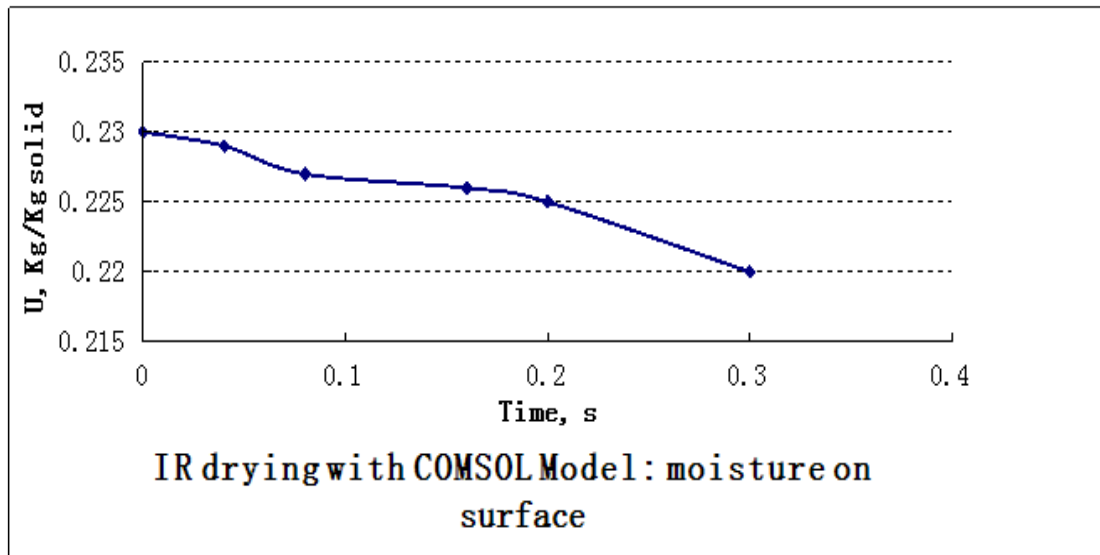


Figure 14. Moisture vs. Time (ir drying in Lampinen, Farkas model: moisture on the surface)

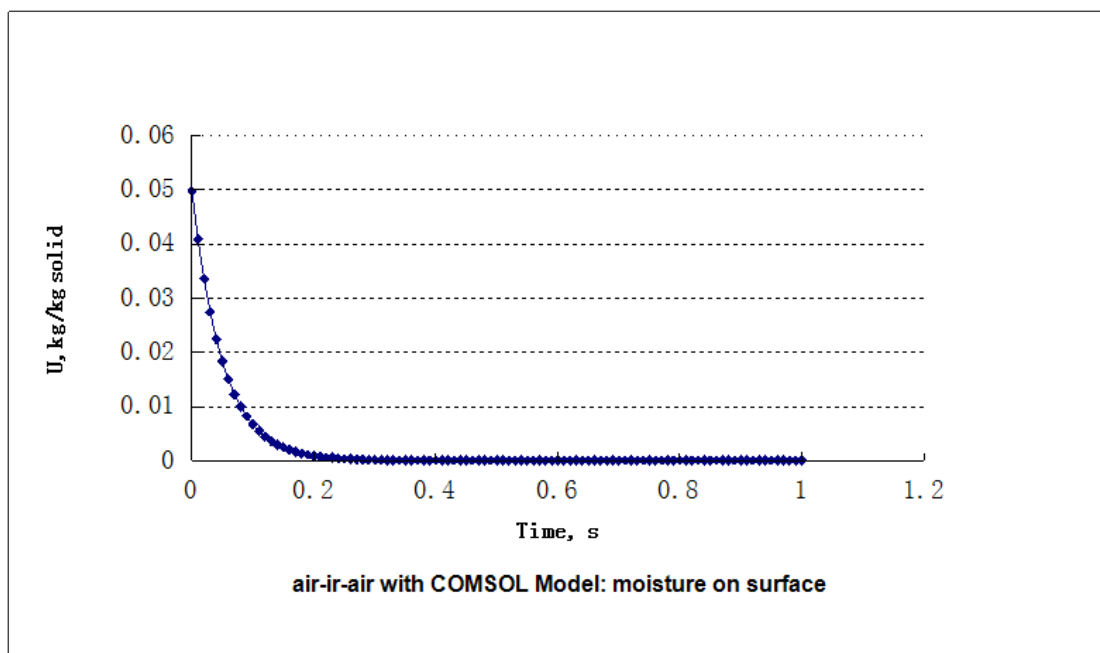


Figure 15. Moisture vs. Time (air-ir-air drying in our COMSOL model: moisture on the surface)

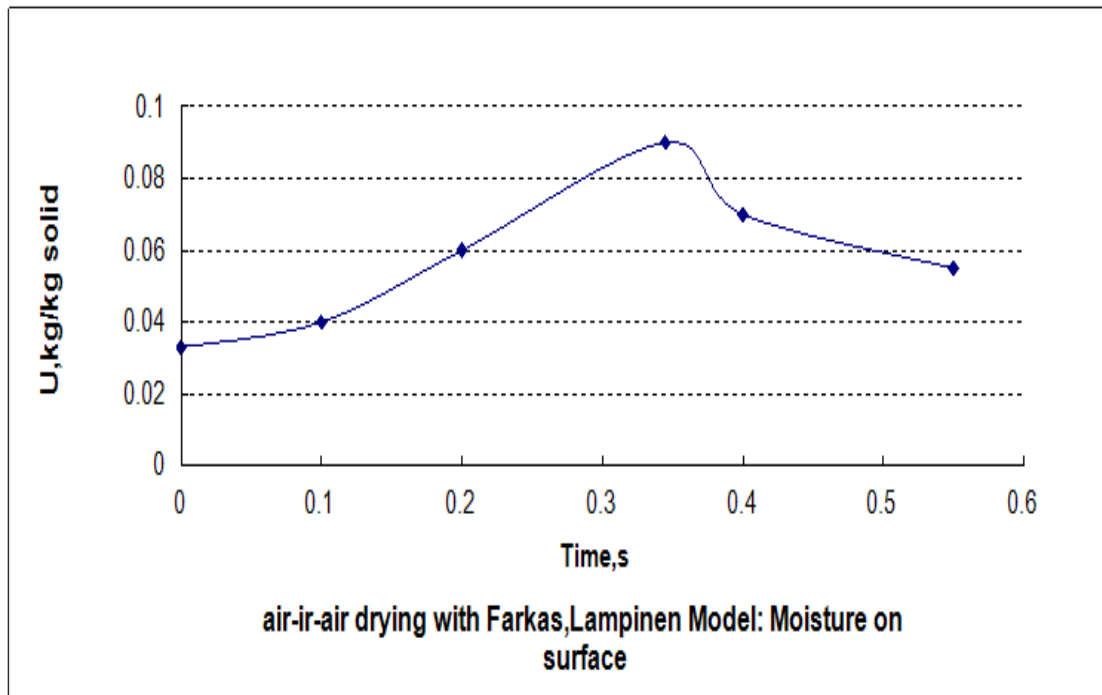


Figure 16. Moisture vs. Time (air-ir-air drying in Lampinen, Farkas model: moisture on the surface)

7.3 Discussion

The COMSOL Multiphysics modeling tool is quite suitable for modeling paper drying process, it can simulate the heat and mass transfer very well. The mathematics model is really convenient for calculation and this tool helped lessen large quantity of calculation work. The mathematics model in the COMSOL is quite accurate and reliable. In one word, the COMSOL Multiphysics modeling tool is very useful in simulating physics phenomenas. It will be a quite good helper in the future studies in modeling and simulating.

A simple model for base paper drying is built, but it is not very satisfying. We compared our model with Lampinen, Farkas model, there are differences between them. We learned about the COMSOL Multiphysics a lot and more detailed knowledge about heat and mass transfer phenomena. Because our models were too simple so that they were not similar to the early models. And our models need to be developed and studied. We need to study much deeper to perfect our modeling study.

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Appendices

APPENDIX 1 Equations

The basic equations are as follow:

Water flux in pores because of capillary flow (Darcy flow)

$$\rho\omega = \frac{k_2}{\nu_2} \frac{\partial p_2}{\partial x} \quad (4)$$

Capillary pressure based on Kelvin equation

$$p_2 - p_{20} = \frac{1}{\nu_2} \frac{RT}{M_3} \ln(\varphi) \quad (5)$$

Sorption isotherm

$$\varphi(u, T) = 1 - e^{-mu^n} \quad (6)$$

Vapor flow by diffusion

$$\rho_3\omega_3 = -\varepsilon_a \frac{p_\beta}{(p_\beta - p_3)} \frac{M_3}{RT} D_{34} \frac{\partial p_3}{\partial x} \quad (7)$$

Heat transfer by convection between sheet and ambient air

$$q = \alpha(T_{ms} - T_4) \quad (8)$$

Mass transfer from paper sheet by evaporation

$$q_{ev} = KIM_3 \ln\left(\frac{P_{4,a}}{P_{4,ms}}\right) \quad (9)$$

Material flux in sheet

$$\rho_l \frac{\partial u}{\partial t} = \frac{\partial}{\partial x} \left(\frac{k_2}{\nu_2} \frac{\partial p_2}{\partial x} + \varepsilon_b \frac{M_a}{RT} D_{34} \frac{\partial p_3}{\partial x} \right) \quad (10)$$

Heat flow in sheet

$$\rho c_p \frac{\partial T}{\partial t} = l \frac{\partial}{\partial x} \left(\varepsilon_b \frac{M_a}{RT} D_v \frac{\partial p_3}{\partial x} \right) + \frac{\partial}{\partial x} \left(\lambda \frac{\partial T}{\partial x} \right) \quad (11)$$

IR radiation

$$r_n = \frac{r_o \eta}{nw} \quad (12)$$

APPENDIX 2 Nomenclature

D	diffusion coefficient
Cp	heat capacity
t	time
ω	velocity
p	pressure
x	length coordinate
R	universal gas constant
T	temperature
M	molar mass
m	constant in isotherm
u	moisture, non-dimensional, water/fiber
n	constant in isotherm, amount of layers in sheet along Z -direction
q	flux
K	mass transfer coefficient
k	water conductivity, water permeability, m ²
l	water latent heat of evaporation
w	machine width
r	radiation energy absorbed in sheet
α	heat transfer coefficient
β	moist air
ε	diffusion resistance coefficient
λ	heat conductivity
η	efficiency in radiation absorption

ρ partial density, mass concentration

ν kinematic viscosity

Indices

o atmospheric

2 water

3 vapor, water

4 air

a drying air

ms moist phase

APPENDIX 3 Models

1 Farkas, Lampinen and Ojala Model

Model assumptions

In this model, the following assumptions have been made:

- Volume fractions and densities are constant, thus no shrinkage is considered.
- The model equations are valid for one or two-sided coated paper; boundary conditions change for each case.
- Phase thermodynamic properties are calculated as weighted averages of the corresponding species' properties that are part of the phase.
- Additional major assumptions made in this model are emphasized in the following discussion.

Model deficiencies

This model lacks refinement in the following aspects:

- It does not account for coating shrinkage, substrate swelling during rewetting, and shrinkage during drying.
- The energy equation does not account for convection effects.
- The mass and energy conservation equations do not account for bound water diffusion.
- Air conservation is not considered, thus pressure distribution within the sheet cannot be predicted for accurate mass flow calculations and prediction of delamination.

2 Bernarda and Bruneau Model

Model assumptions

The following lists the main assumptions in this model.

- While the model accounts for temperature distribution within the base stock, it assumes that the temperature remains constant within the coating thickness.
- Liquid drains from the coating to the base stock as long as there is mobile water in the coating.
- Up to the solid immobilization, evaporation occurs on the surface of the coating.
- After the solid immobilization, evaporation from the coating is calculated according to a descending front model, based upon the calculation of the volume occupied by the liquid phase.
- When the evaporation front reaches the base stock, the coating is permeable for the vapor that is being produced in the base stock.
- Base stock materials properties are constant in the thickness direction, being function of the base stock average moisture content and temperature.
- Empirically, evaporation in the base stock is assumed to be evenly distributed through its thickness.
- In the calculation of vapor flow through the base stock, the average diffusion depth of vapor is empirically assumed to be half of the thickness of the base stock.

Model deficiencies

The model lacks refinement in the following aspects:

- Energy equation is rather incomplete, since it does not have the convection terms.
- Need to account for binder diffusion (migration) through the use of mass conservation equations for all the species present on the system. Binder concentration in the evaporation front and the corresponding mass diffusion are the result of water evaporation from the coating. These events are not considered in the model.
- Material properties should be calculated as a function of the local temperature and moisture content.
- Diffusion depth should be calculated by evaluating competing capillary pressures in the paper and the coating.
- Radiation heat transfer, which is treated as a linear function of the material's base weight, should be accounted by an exponential absorption coefficient.

3 Bernarda and Bruneau Model

Model assumptions

The principal assumptions made in this model are the following:

- Even though binder migration modifies the intrinsic density of the solid phase, it is assumed to be constant. Bernarda and Bruneau (1995) note that binder deposition influence on the solid phase intrinsic density is rather small.

- During the drying process, the coating is assumed to be isothermal which is the weakest assumption of this model since its temperature changes during drying.
- Interaction with the base stock is considered with a simple Dirichlet boundary condition.
- Evaporation is accounted by an empirical expression of the vapor flow as a function of time.
- The mass conservation of binder at the interface with the base stock sets the binder flow rate to zero. This might be true for particulate binder for which its flow is restricted by the base stock fibers. However, it is not necessarily the case for soluble binder, which can flow with the liquid phase without restrictions.

Model deficiencies

The model lacks refinement in the following areas:

- Needs to include the energy equation to find the temperature profile during drying. Paper does not behave isothermally during drying.
- Transport properties should be function of local temperature and moisture content.
- Vapor transport inside the coating should be accounted.
- Evaporation should be modeled using Fick's Law.
- Capillary forces and Darcy's Law should be used for modeling water drainage into the base stock.
- Binder migration model is empirical. It should be modeled using Fick's law. Soluble binders do migrate with the water into the base stock. Particulate binder might not. This model precludes any binder migration into the base stock.

4 Rajala and Karlsson Model

Model assumptions

The following are the main assumptions of the model:

- Coating is formed of a homogeneous material, no binder migration is accounted.
- Air is not considered in the model, thus, no total pressure is calculated.
- Material properties of the coating and paper are calculated from the properties of the different components according to the proportional weight of each species. It is not clear whether the properties are calculated at local or average temperature and moisture contents.
- No convection effects are considered in the energy equation.
- Liquid water flow and base stock rewetting are accounted by capillary and Darcy's Law.
- Water evaporation is accounted by a mass transfer coefficient, which is not explicitly defined.

- Vapor diffusion is accounted by Fick's Law.
- IR radiation is evenly absorbed throughout the coating and the base stock.

Model deficiencies

- The model does not account for binder migration within the liquid and binder deposition in the solid phase.
- Air should be considered in the mass conservation equations for the model to be able to predict the pressure distribution within the domain.
- Energy equation should account for convection effects.
- IR radiation should be accounted for by an exponential function, through an appropriate absorption coefficient.
- Water and binder drainage to the base stock is not properly accounted
Shrinkage of the coating is not accounted for.

5 Nowicki Davis and Scriven Pan, Davis and Scriven Models

Model assumptions

- Coating is modeled as a network of voids and connecting passages in a microscopic scale.
- The irregular (coating) network is described as a regular network with the same average coordination.
- Pore passages vary in cross section along their length. This is modeled using bi-conical pore passages.
- To account for variations in pore space throughout the coating, the cone angles and the radii of the constrictions (pore throats) are drawn in the model from statistical distributions typical of paper coating.
- In initial state pore space is full of liquid and all menisci are flat.
- Binder convects to and concentrates at evaporating menisci.
- Binder diffuses away from these menisci as concentration gradient is established.
- Evaporation is isothermal.
- When the saturation concentration is reached, binder deposits as a solid in the base structure of the coating.

Model deficiencies

- The model should include the energy equation, to be able to predict temperature distributions in the liquid and the solid phases.
- Water drainage to the base stock should be included.
- The two dimensional model seems better to describe the binder migration.

APPENDIX 4 Figures

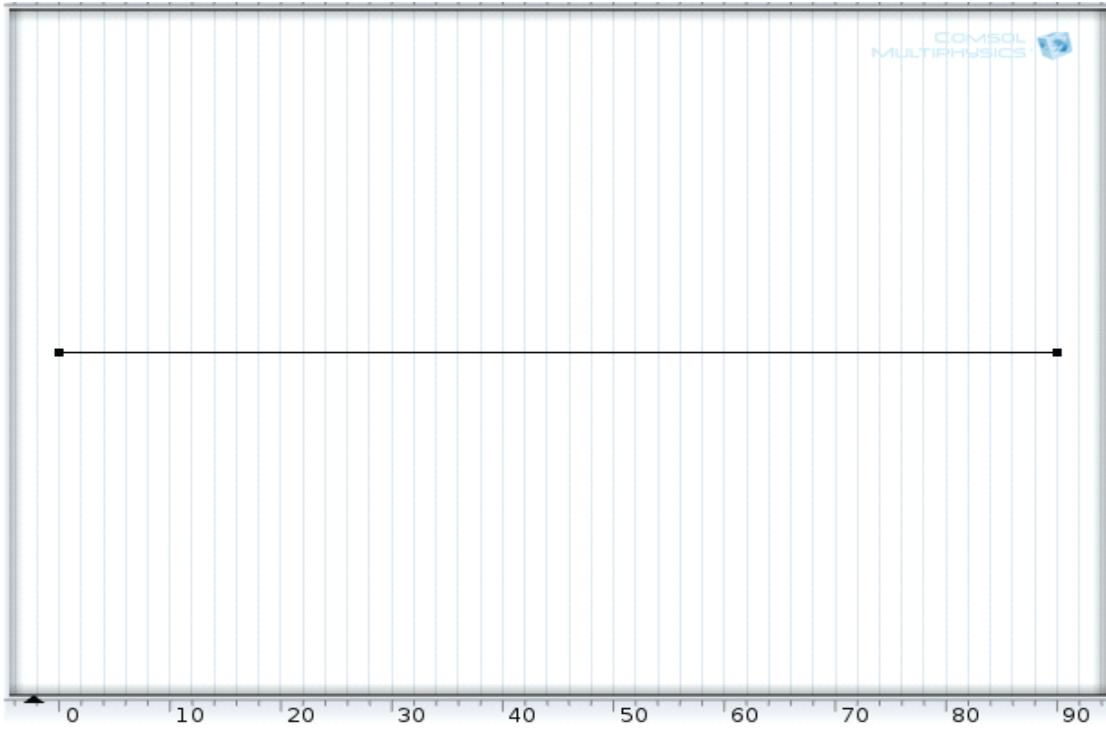


Figure 17. Definition (the left endpoint is 0 μm and the right endpoint is 90 μm)

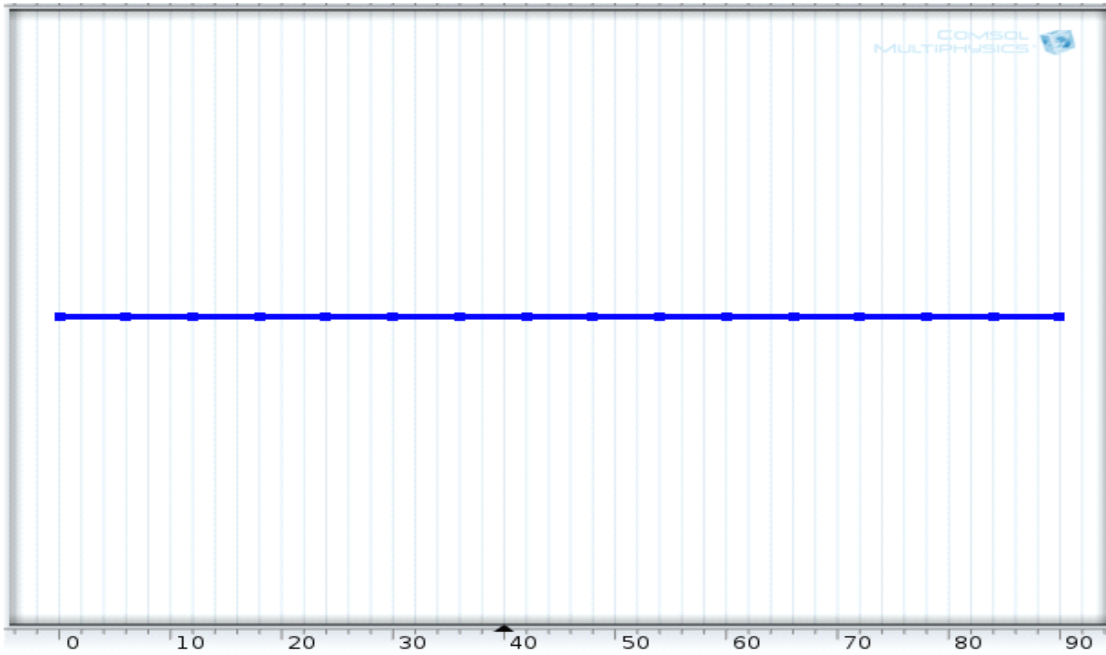


Figure 18. Mesh

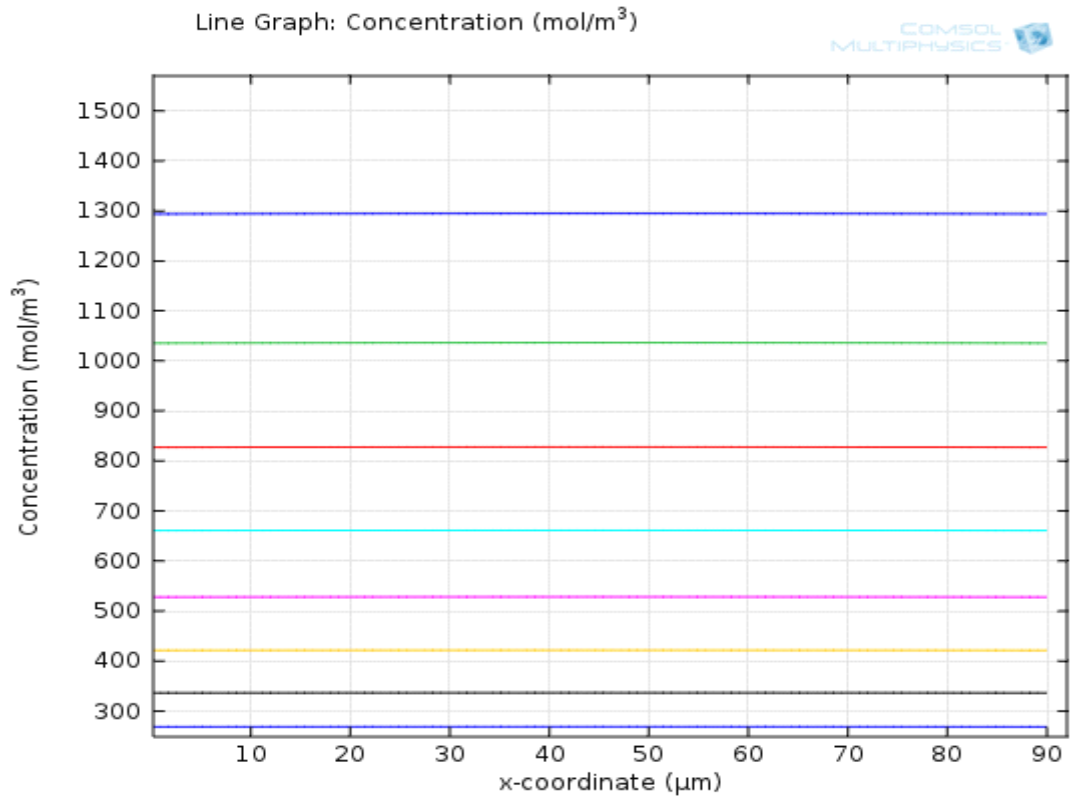


Figure 19. Concentration on the surface

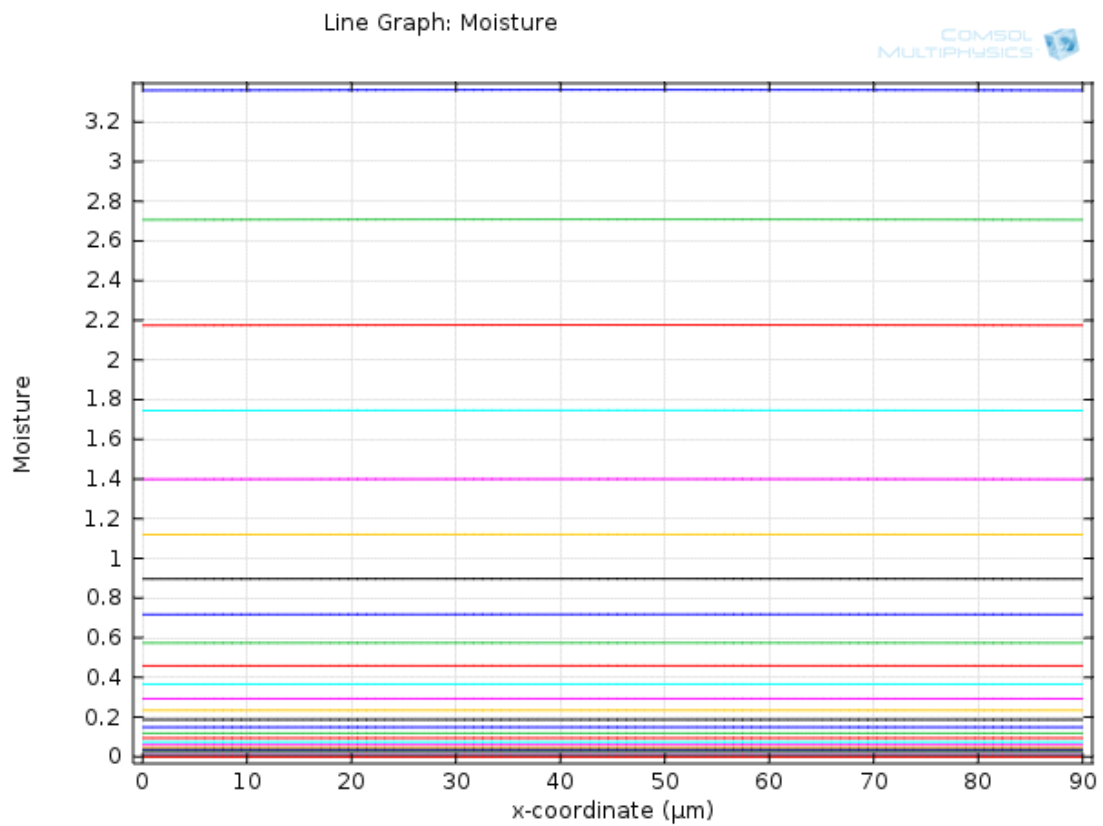


Figure 20. Moisture on the surface

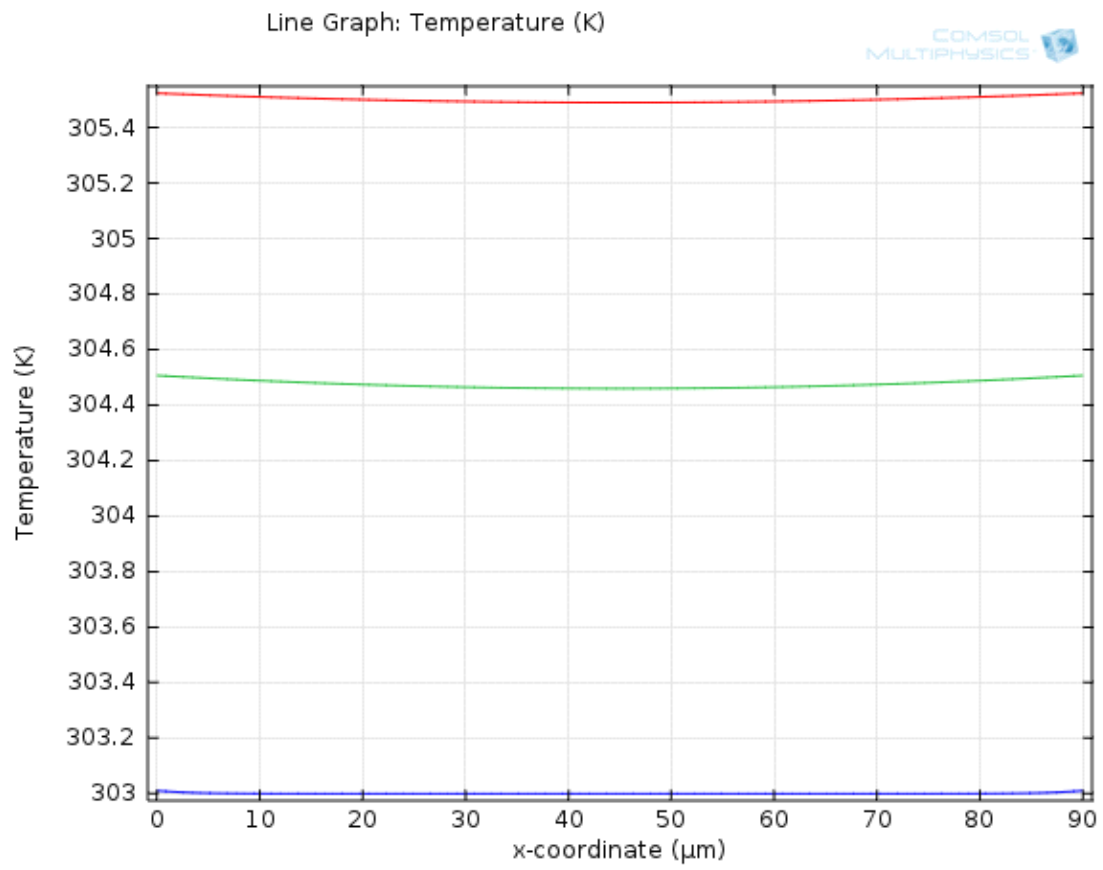


Figure 21. Temperature on the surface