

# Adding milk properties models for process simulation in Aspen Plus v. 8.2

Complementary information to the article :

*Madoumier, M., Azzaro-Pantel, C., Tanguy-Sai, G., Gésan-Guiziou, G. (2015). Modelling the properties of liquid foods for use of process flowsheeting simulators : Application to milk concentration. Journal of Food Engineering, 164, 70-89.*

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## Introduction

In the paper « Modelling the properties of liquid foods for use of process flowsheeting simulators: Application to milk concentration », milk properties models are added to the Aspen Plus (Aspen Technology, Inc., Burlington, United States) simulation software, so as to perform process simulations for the concentration of milk. The precise method used to add these models to Aspen Plus is not given in the paper, hence this complementary information.

## Creating custom components

In Madoumier et al. (2015), milk is modeled as a mixture of 5 components: water, fat, proteins, carbohydrates, minerals. Water is already present in the Aspen Plus components database, whereas the remaining 4 components do not exist in the database. Therefore, they are added to Aspen Plus as user-defined components.

In Aspen Plus, it is possible to add user-defined components as “conventional” or “non-conventional” components. The 4 “bulk” components of milk dry matter (fat, proteins, carbohydrates, minerals) were added as conventional components. Indeed, the modeling of liquid mixture properties of milk, as described in the next section, would not be possible if milk dry matter components were modeled as “non-conventional” components in Aspen Plus.

A number of hypotheses were considered in order to fill the physical properties of the user-defined components, since conventional components require some information for the Aspen Plus thermodynamic engine to work. Table 1 indicates the naming and the molecular weight of the components as set in Aspen Plus. The saturated liquid is selected as the reference state, since the property models refer to the liquid phase. For each component, the reference temperature for liquid enthalpy is 25°C and the reference enthalpy for the liquid state at the reference temperature is 0. For more information regarding milk user-defined components, please refer to Madoumier et al. (2015).

Table 1: Naming and properties of milk dry matter components as defined in Madoumier et al. (2015)

Milk bulk component	Naming in Aspen Plus	Molecular weight (g.mol <sup>-1</sup> )	Reference state
Fat	MILKFAT	1 350 000 000	Liquid
Proteins	MILKPROT	16 300 000	Liquid
Carbohydrates	MILKCARB	342	Liquid
Minerals	MILKASH	50.13	Liquid

## Modifying properties method

As stated in Madoumier et al. (2015), the main thermodynamic mixture properties in Aspen Plus are replaced by external Fortran programs, i.e. subroutines coded by Madoumier et al. These Fortran programs contain the properties models described in Madoumier et al. (2015). Table 2 indicates the milk properties added to Aspen Plus and the corresponding thermodynamic properties and Fortran files. The Fortran files are given with this document.

Two things are necessary for Aspen Plus to take these Fortran subroutines into account when performing simulations:

- When setting the thermodynamic (physical) properties in the main Aspen Plus interface (*Methods/Selected Methods*), the Fortran subroutines must be specified. Whatever the properties method selected (default methods such as “IDEAL” or a custom user method), the “Route ID” must be modified in the “Routes” tab. For example, for the specific heat capacity of milk, the corresponding physical property is the Mixture liquid molar enthalpy, which is labeled “HLMX” in the “Routes” tab. In the “HLMX” row, the “Route ID” must be set to “HL2USR”, which is the name of the corresponding Fortran subroutine.
- A Fortran compiler needs to be installed, so that the Fortran subroutines can be used by Aspen Plus. For more information regarding the compiler, please refer to the relevant Aspen Plus documentation (Aspen Technology, 2011).

These requirements are valid for Aspen Plus version 8.2.

Table 2: Milk properties, corresponding thermodynamic properties and corresponding Fortran files added to Aspen Plus

Milk property	Aspen Plus thermodynamic property	Aspen Plus Route ID	Fortran file
Specific heat capacity	Mixture liquid molar enthalpy	HLMX	HL2USR.F
Boiling point elevation	Liquid phase activity coefficient	GAMMA	gmu.f
Density	Mixture liquid molar volume	VLMX	VL2USR.f
Thermal conductivity	Mixture liquid thermal conductivity	KLMX	KL2USR.f
Viscosity	Mixture liquid dynamic viscosity	MULMX	MUL2USR.f
Surface tension	Mixture liquid surface tension	SIGLMX	SIG2USR.f

## Disclaimer

This complementary information requires a minimal knowledge of the Aspen Plus software. For any missing information, missing files and/or mistakes, please contact me via my professional e-mail address. Otherwise, try my LinkedIn profile: <https://www.linkedin.com/in/martialmadoumier/>

## References

- Aspen Technology (2011). *Aspen Plus – User Models*. Aspen Technology, Inc., 200 Wheeler Road - Burlington, MA 01803-5501 – USA. Aspen Plus version 8.6.
- Madoumier, M., Azzaro-Pantel, C., Tanguy-Sai, G., Gésan-Guiziou, G. (2015). *Modelling the properties of liquid foods for use of process flowsheeting simulators : Application to milk concentration*. Journal of Food Engineering, 164, 70-89.