

# **Rigorous dynamic simulation of cryogenic distillation of hydrogen isotopologues in the fuel cycle of a thermonuclear reactor based on UV-flash**

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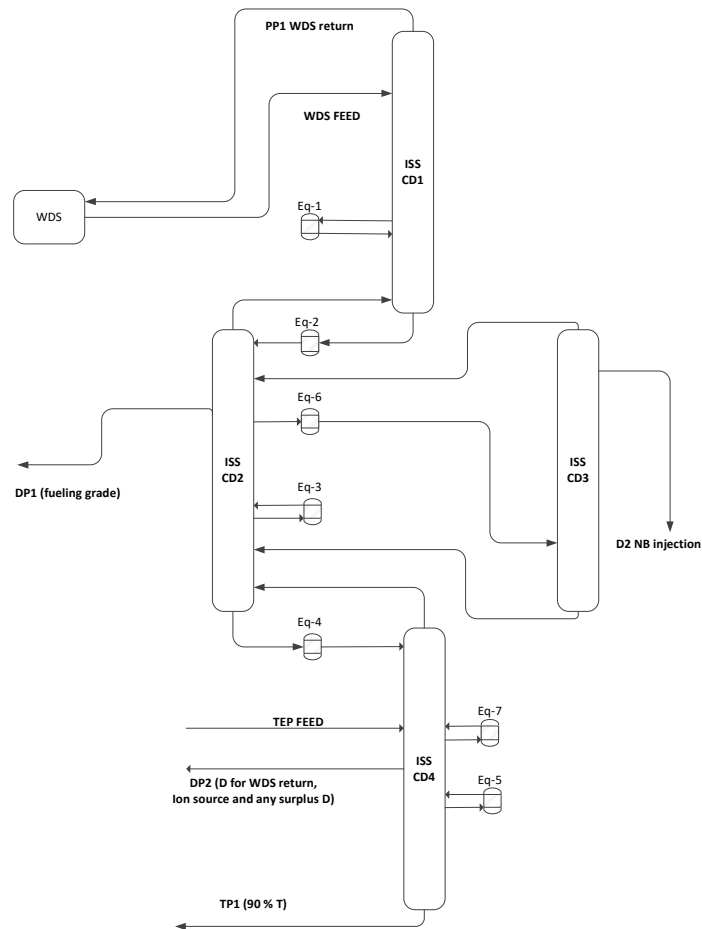
## **Abstract**

Operation of the fuel cycle of a thermonuclear fusion reactor naturally leads to accumulation of surplus protium but in some cases it can also lead to accumulation of surplus deuterium. Both surplus protium and deuterium have to be separated, detritiated and discharged to the environment normally passing a final detritiation stage based on either the LPCE (liquid phase catalytic exchange) or water distillation process. A concept of a multicolumn cryogenic distillation system capable of discharging time varying surplus of deuterium is presented in the article together with its dynamic model. The model is based on a UV flash formulation and equation of state (EOS) thermodynamic model for hydrogen isotopologue mixtures. The UV (internal energy - volume) formulation of thermodynamic state although fundamental for the constant volume system has not been used widely in transient simulations, in particular, for distillation dynamics modelling other approaches are much more common. At the same time in helium cryogenics the UV formulation has reached a wide usage in large scale dynamic simulations. It is known from the literature that a UV formulation of the distillation problem is very challenging for a numerically stable implementation. We present our findings on the sources of numerical instabilities and approaches to cope with it.

## **Isotope separation in the fuel cycle of a thermonuclear reactor and accumulation of deuterium**

Operation of the fuel cycle of a thermonuclear fusion reactor naturally leads to accumulation of surplus protium but in some cases it can also lead to accumulation of surplus deuterium. These cases are the flowing. First every concept of a thermonuclear reactor fuel cycle comprises a water detritiation system, in some cases this system is a very large one as it is the case at ITER. Operation of water detritiation system (WDS) leads to accumulation of D naturally present in water at ~ 145 (ppm) levels. Clearly with e.g. 50 (kg/h) water detritiation capacity approximately 0.4 (mol/h) of D<sub>2</sub> will be accumulated in the fuel cycle. If any regular injection of gas bottle deuterium for any purpose is done this deuterium becomes contaminated with tritium and adds the surplus of deuterium in the fuel cycle.

For ITER the concept of the Isotope Separation System (ISS) was first time finalized in July 2001 when the ITER Technical Basis Document was published on the basis of numerous Design Description Documents (DDD)s developed by that time [1]. The concept was developed in several iterations described in [2][3][4]. The schematics below show the final configuration this concept henceforth referred as ITER 2001 ISS [5]:

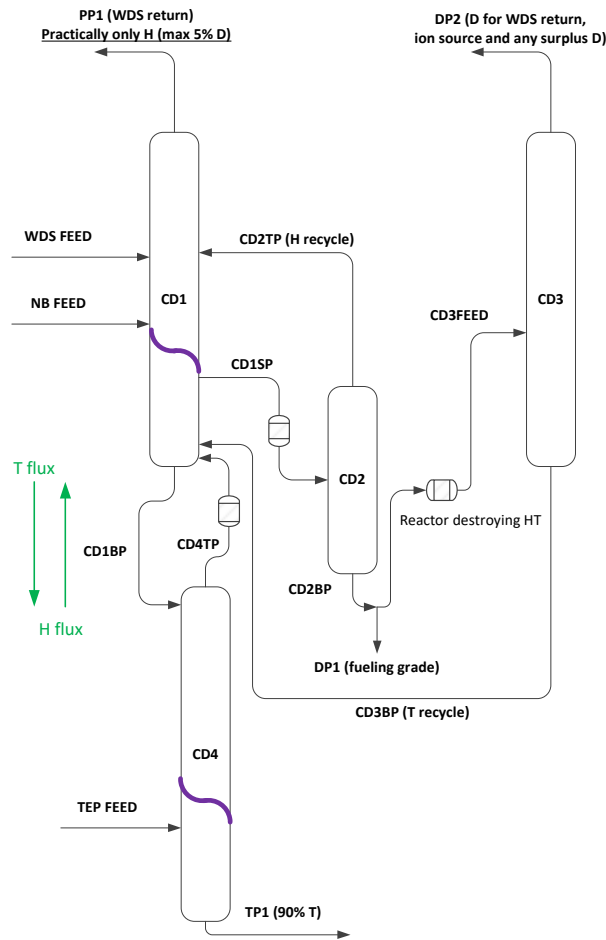


**Figure 1. Configuration of ITER 2001 baseline ISS concept**

In [1] the following description is given. The column cascade consists of four distillation columns (CD1, CD2, CD3 and CD4). The purpose of the first column (CD1) is to remove tritium from predominantly protium-rich streams and to produce a virtually tritium-free protium stream as the overhead product. The function of the second column CD2 is to separate H and D from the CD4 overhead stream, and produce a partially-purified D2 stream which is used for gas fueling and as the feed to the third column CD3. CD3 removes tritium and protium from the deuterium for NB injector source gas. The bottom product of CD2, a D2-DT mixture stream, is fed into the high-tritium-column CD4, which also receives elemental hydrogen separated in the tokamak exhaust processing system from the plasma exhaust stream.

Clearly if there is a significant accumulation of both surplus protium and deuterium they have to be separated, detritiated and discharged to the environment normally passing a final detritiation stage based on either the LPCE (liquid phase catalytic exchange) or water distillation process. Potential accumulation of deuterium and the necessity to get rid of this surplus deuterium have never been fully addressed in ITER 2001 ISS because both aforementioned sources of surplus deuterium were considered small. In particular deuterium for NB injector source gas taken from CD3 in ITER 2001 ISS had about 75 ppm of T in it as it was never intended to be returned to WDS for final detritiation. Return flow to WDS from CD1 “protium return” had just 1.2 atomic % of D.

Reconsideration of ISS concept was started with the adaptation of commercial software Aspen Plus to the calculations of cryogenic distillation cascades. Properties of hydrogen isotopes were put into Aspen Properties database and correct calculation of vapor liquid equilibrium in strict accordance with the Sherwood-Souers thermodynamic model [8] was implemented using an external Fortran user-supplied function in Aspen Properties. As a result a robust way to make steady state calculations for any configurations of cryogenic distillation cascades was established at ITER. Then several options were investigated using steady state calculations in Aspen Plus. Steady state model of ITER 2001 ISS was reproduced. The main problem identified was inability to discharge significant amounts of D with the “protium return” flow from CD1. As soon as concentration of D in this stream goes above ~5% tritium concentration goes above acceptable. This is results of very low difference in volatility of HD and HT hydrogen isotopologues. If we need to discharge with “protium return” flow much of HD we will always see too high HT concentration in the same flow. The solution proposed is to separate points where very pure H and D are withdrawn and provide very deep detritiation of one deuterium product that it can be sent to WDS for final detritiation and discharge to the atmosphere [12]. The proposal is presented below:



**Figure 2. Possible new configuration of ITER ISS concept**

We still have 4 columns in the proposed new configuration but the connections are somewhat simplified. In this proposal CD1 and CD4 are still connected by the two way connection. Such a connection has the capability of transferring all H from CD4 up to CD1 and finally WDS and simultaneously provides flux of T from the bottom of CD1 down to CD4 to extract part of T present in NB (Neutral Beam) feed and WDS feed (see Fig 2.). From the top of CD1 column practically pure HH is taken with less than 5% D in it. This provides a very deep detritiation of this stream. Low purity deuterium (DP1) is produced from a side stream taken from CD1 column that is predominantly D with low H concentration. In CD2 protium is separated from D and protium is recycled back to CD1 with CD2TP stream. Between CD2 and CD3 a room-temperature reactor promoting isotopic self-equilibration destroys traces of light DT molecules converting T to heavy DT isotopologue that is concentrated in the bottom of CD3 and recycled back to the reboiler of CD1. Very pure D with less

than 10 ppm of T is produced with the top stream DP2 of CD3. This product can be used for both ion source of the neutral beam injector and for discharge to WDS for final detritiation before rejection to the environment.

The recycle of protium from CD2 and change from a side column for pure D production to a dedicated stand along column CD3 in the new proposal are the key features that provide capability to work with WDS feed stream of 280 (mol/h) as in [1] with up to 50% of D in it.

## **Rigorous dynamic simulation of cryogenic distillation of hydrogen isotopologues based on UV flash**

Cryogenic distillation of hydrogen isotopes has been the leading separation method applied when a high throughput high concentration tritium separation process is needed as in the fuel cycle of a large thermonuclear reactor. There is a wealth of publications on the transient modeling of this process e.g. [4][6][13][14] and many others. However, to the best of authors' knowledge, in all of them the model is based on the use of bubble flash (constant pressure) calculations of vapor liquid equilibrium. The assumption of constant pressure is natural for columns connected to the atmosphere or to a source of constant pressure that can be e.g. a vacuum manifold as it is done for water distillation at ~20 kPa for the production of oxygen isotopes. However for most of the distillation facilities including cryogenic distillation for hydrogen isotopes separation it is impossible to have any connection to a source of stable pressure. The absolute pressure in them is controlled by the balance of heat sources, most importantly heating in the reboiler, and cooling in the condenser. A distillation column not connected to a source of constant pressure is a constant volume open system with natural state variables molar amounts of the components and internal energy in each volume that is on each tray [26] this selection of state variables in combination with rigorous UV-based phase equilibrium calculation (UV flash) we henceforth call the UV approach. As discussed at length in [23] the UV approach is the most rigorous approach to transient distillation modeling that still uses the concept of the theoretical tray.

The argument provided in support of fixed pressures in the condensers is that pressure control is normally rather tight. However if a cryogenic distillation facility faces very significant variations in the flow rate and composition of the feed flows it seems reasonable to have both the thermodynamic and hydraulic response of the system modelled fully rigorously for a detailed transient analysis. This idea was the main driver for the effort presented in this article.

It should also be noted that for single component fluids when the UV-based phase equilibrium calculation (henceforth UV flash) can be replaced by a table lookup in an internal energy-density table

this UV approach has been successfully used in CRYOLIB [18][19] and FLUIDAPRO [22] fluidic libraries for EcosimPro. For multicomponent fluids it was also reported e.g. in [24] and in [23] it was applied to distillation in particular. The straightforward UV approach in [23] was augmented by the use of local thermodynamic model that was the most evident way to accelerate multicomponent thermodynamic calculations when parallelization of computations was not readily available.

Thermodynamic calculations are extremely well parallelizable by their nature as results of each computation is a small set of output results that depends on a small set of input data and each thermodynamic equilibrium calculation (flash calculation) is independent of all the others. Numerous iterations made on a small set of data make equilibrium calculations compute-bound also facilitating parallelization. These factors naturally make phase equilibrium calculations amenable to massive parallelization. A good review of this topic is provided in [17] that describes the use of modern graphical accelerators for vapor-liquid equilibrium calculations. Nowadays a single high-end consumer CPU can have up to 32 cores and the enormous development of computing power for High Performance Computing (HPC) applications in science and engineering often leaves some idling fraction of their computing power available at a marginal or no cost for process design calculations. Consequently the brute force UV approach when a multicomponent UV flash calculation is done rigorously for each tray at all times has become a more viable option now when the much slower performance of it can be offset by the availability of hardware for parallel computations.

Probably the first commercially available thermodynamic system that implemented full thread safety for multicomponent thermodynamic equilibrium calculations including the UV specification and, consequently, capability to be readily parallelized using e.g. OpenMP was KBC Multiflash starting from version 6.2 issued in 2016, technical details about the approach to parallelization can be found in [25]. Clearly a model of a distillation system could have been implemented in standard programming language like C++ but we decided to use an equation-oriented modeling system EcosimPro that has been used successfully at CERN, ITER and CEA for many years for the modeling of large scale cryogenic systems [18][19][21][20]. This decision was based on the flexibility provided by EcosimPro and the multitude of features already implemented in EcosimPro that otherwise will have



to be implemented anew. It was also supported by a rather wide use of similar equation-oriented systems in the chemical engineering domain starting for the first commercially available equation oriented modeling system SpeedUp [29][30] that has evolved into Aspen Custom Modeler/Aspen Plus Dynamics and its further development gPROMS [27][28].

In this article we present our efforts aimed at providing an equation of state based thermodynamic model for hydrogen isotopologues, a software connection between EcosimPro and Mutiflash and results of first tests of them on a single distillation column of 110 theoretical trays

All tests and their timings presented in this article were made on a dual Intel Xeon workstation with two E5-2670 CPUs (16 physical cores in total) running at 2.6 GHz. Experimental version 6.1.30 of EcosimPro software was used for all tests.

### **Equation of state thermodynamic model for hydrogen isotopologues**

De-facto standard vapor-liquid equilibrium (VLE) model for the hydrogen isotopologues is the Sherwood-Souers model [8] that is an activity-fugacity model. Activity-fugacity thermodynamic models for VLE in general are not compatible with the UV formulation. Consequently an equation of state (EOS) VLE model for hydrogen isotopologues was developed based on pseudo-data generated from the Sherwood model. As additional sources of information data from the book by Soures [9] were used for all isotopologues but for HH and DD [10] data were used as more precise. KBC Multiflash includes a wide range of EOS models but many are not appropriate for the current application. Accurate wide-ranging data and EOS are only available for HH and DD [10] so models such as GERG2008 that depend on high-accuracy EOS for each pure component in a mixture are not applicable. Generalised models such as BWRS and LKP [11] are not parameterized for quantum gases and low temperatures.

In order to fit binary interaction parameters (BIPs) for Multiflash models based on pseudo-data from the Sherwood model it is essential that the pure component vapour pressure (VP) correlations reproduce the Souers VP values as closely as possible. However, the Souers correlations are simple Antoine equations with limited ranges of validity and, in particular, they are not consistent with the critical point values. If the Souers VP correlations are used in Multiflash the advanced cubic equation of state (EOS) models cannot accurately reproduce the VPs because of this inconsistency. Therefore, it has been necessary to refit the VP of all components using Wagner-type VP correlations (Multiflash vapour pressure equations 1 and 3 defined in [11]) that correctly reproduce the critical point. Then pseudo-data generated from the Sherwood model has been used to regress BIPs for all the 15 binary systems formed by the six hydrogen isotopologues. Temperature-independent BIPs have been used in all cases because the VLE data covers a quite narrow temperature range between 20 (K) and 27 (K) and it is required to apply the same model up to around 600 (K).

The recommended Multiflash model for representing the VLE of Hydrogen isotopologues is the Redlich-Kwong-Soave Advanced (RKSA) model [11]. The perfect gas heat capacities of all components have been fitted to Multiflash equations that reproduce the data used to within 1% for most substances with a maximum deviation of 1.5% for DD. The combination of the perfect gas heat capacity correlations and the RKSA model should provide reasonable predictions of thermal properties from cryogenic conditions to 600 (K) as required. The enthalpy change on evaporation of HH and DD, the only substances for which high accuracy values are available, are well reproduced by the recommended RKSA model and we can expect that for other 4 isotopologues enthalpy change on evaporation are rather accurate.

The RKSA model developed can be used with any of the flash calculations available in Multiflash including the UV flash.

**Development of a software link between EcosimPro and KBC Multiflash and multicomponent library of basic models**

KBC Multiflash provides two Application Programming Interfaces (APIs) in Fortran and in C/C++. In order to make parallel calls to flash routines in a thread safe way the new C/C++ interface of KBC Multiflash should be used [25] An intermediate layer DLL providing easy to use abstraction of Multiflash C/C++ interface was developed at ITER. Several Multiflash streams are supported so we can have several parts in one simulation using different sets of components and different thermodynamic models but the intermediate layer is limited to 2 phases gaseous and liquid that is sufficient for all envisaged applications at ITER. The principal idea of the intermediate layer was to have just a single call to UV flash in any volume that also returns all the data necessary for reporting to the user (e.g. molar fractions) and for the calculation of flow rates in resistive components attached to this volume component as described further.

One of the key design decisions in the development of an equation oriented library of components is to define a port type. Ports in EcosimPro and other equation-oriented languages serve as links between any two components for information exchange. The values of the variables exposed through these elements from one component to another. Usually for fluidic simulations sequences of volume-resistance-volume model are recommended as they avoid creation of algebraic equation systems and make simulation more robust and convertible to an ordinary differential equations (ODE) system. Volumes or pressure setters in our library have molar holdups of substances and total energy in them as state variables and in a UV flash and subsequent calls to property evaluation functions calculate all intensive and (if requested) transport properties that is done in a single call to the intermediate layer DLL. This volume-resistance-volume pattern makes desirable to have exposed in volume ports all information needed for the resistance to calculate flow rate between the two volumes that is fluid mass density and viscosity. Clearly some types of flow resistances need to make thermodynamic calculations on their own e.g. flashing valves but in low pressure drop resistances information provided by adjacent ports is sufficient.

The structure of port type used in the multicomponent library for EcosimPro based on Multiflash thermodynamic software is shown in table.

**Table I Structure of Port Type Used in the Multicomponent Library for EcosimPro**

<b>Construction parameter</b>	
nc	components of Multiflash Fluid
ncon	Number of connections
<b>Information exposed in port about the state in the volume*</b>	
P_inV[ncon], (Pa)	Pressure from volume equal equations
H_inV[ncon], (J/mol)	Enthalpy from volume equal equations
Z_inV[ncon,nc]	molar fractions from volume equal equations
<b>Additional information calculated in the volume and reported in the port for the possible use in resistive element**</b>	
Rho_inV[ncon], mol/m <sup>3</sup>	molar density from volume equal equations
Mw_inV[ncon], g/mol	averaged molecular weight used to get mass density
LiqVolFrac[ncon],	liquid volume fraction from volume equal equations
<b>Values calculated in resistive component***</b>	
F[ncon], (mol/s)	molar flow rate in the moving fluid
H_flow[ncon], (J/mol)	molar enthalpy in the moving fluid
Zi_flow[ncon,nc]	molar fractions in the moving fluid

\* - the set of information exposed (minimum for resistive element to be aware) must be sufficient for a resistive element to obtain all information about fluid with the use of calls to thermodynamic properties routines if this is needed (e.g. in a flashing valve).

\*\* - the set of additional information reported in the port should provide all information needed for the simplest and very common types of hydraulic resistances – K loss factor and the pressure drop

correlation in a distillation column [16]. This type of resistance should not calculate any physical properties inside its code, all must be available through the ports.

\*\*\*- this set of values must be fully sufficient but not exceed what is needed for mass and energy balance equations inside the volume model. Additional information like volumetric flow rate can reported by the resistive component is needed.

An important feature of the developed multicomponent library is the availability of a gas only UV calculation. In many cases it is a-priori known that a volume will never work in two phase region. For a thermonuclear reactor most of the systems work relatively low pressures and room or higher temperatures with so-called non-condensable gases that can be considered ideal gases. In the developed library of models and the intermediate layer DLL it is possible for the user to set a flag in a volume model that this volume is a gas-only volume. In this case in the intermediate layer instead of calling Multiflash UV flash the procedure finds using the Bent's method the temperature of the gas from the known amounts of components and internal energy using Multiflash API function returning the perfect gas enthalpy and entropy for each component of the mixture and the ideal gas law. Such a calculation is at least 100 times faster than UV flash and results are very close to full UV flash calculations as the same perfect gas thermodynamic data are used.

It should be mentioned that a similar project aimed at the creation of a software interface from equation-oriented software Dymola to KBC Multiflash was undertaken before in [15] but not specifically for distillation modelling and without parallelization of calculations that was not available at that time in both Dymola and KBC Multiflash.

## Numerical issues and their resolution

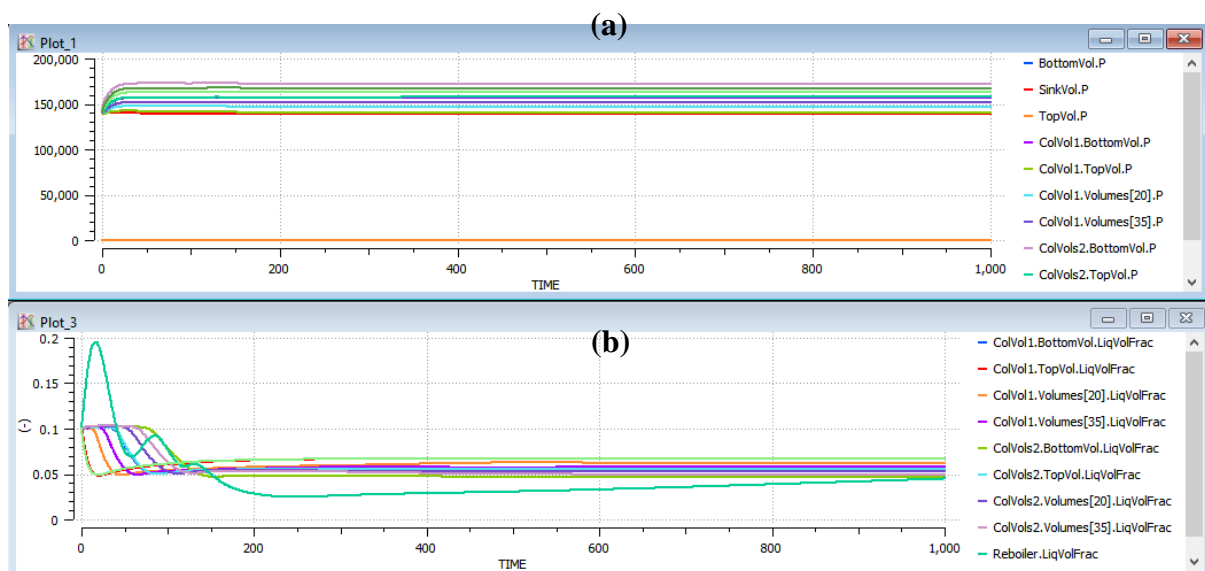
All transient formulations of the distillation problem produce stiff system of ODEs. UV formulation produces a particularly stiff system [23]. Consequently a stiff ODE solver is needed and in this work two solvers were used a sparse version of well-known CVODE in EcosimPro and ode15s solver in Matlab. It should be noted that unlike SpeedUp/Aspen Custom Modeler and gPROMS, EcosimPro just like ode15s in Matlab does not produce analytical expressions for Jacobian evaluation but relies exclusively on forward finite differencing to evaluate the elements of the Jacobian.

During the development of aforementioned software interface and for testing purposes we used a test system of six closely boiling hydrocarbons: Pentane, Hexane, 2-Methylpentane, 3-Methylpentane, 2,2-Dimethylbutane, 2,3-dimethylbutane with Redlich-Kwong-Soave (RKS) equation of state (henceforth the hydrocarbon system). This allowed us to separate general, the fundamental performance and robustness issues from the issues specific to the cryogenic case of the hydrogen isotopologues system.

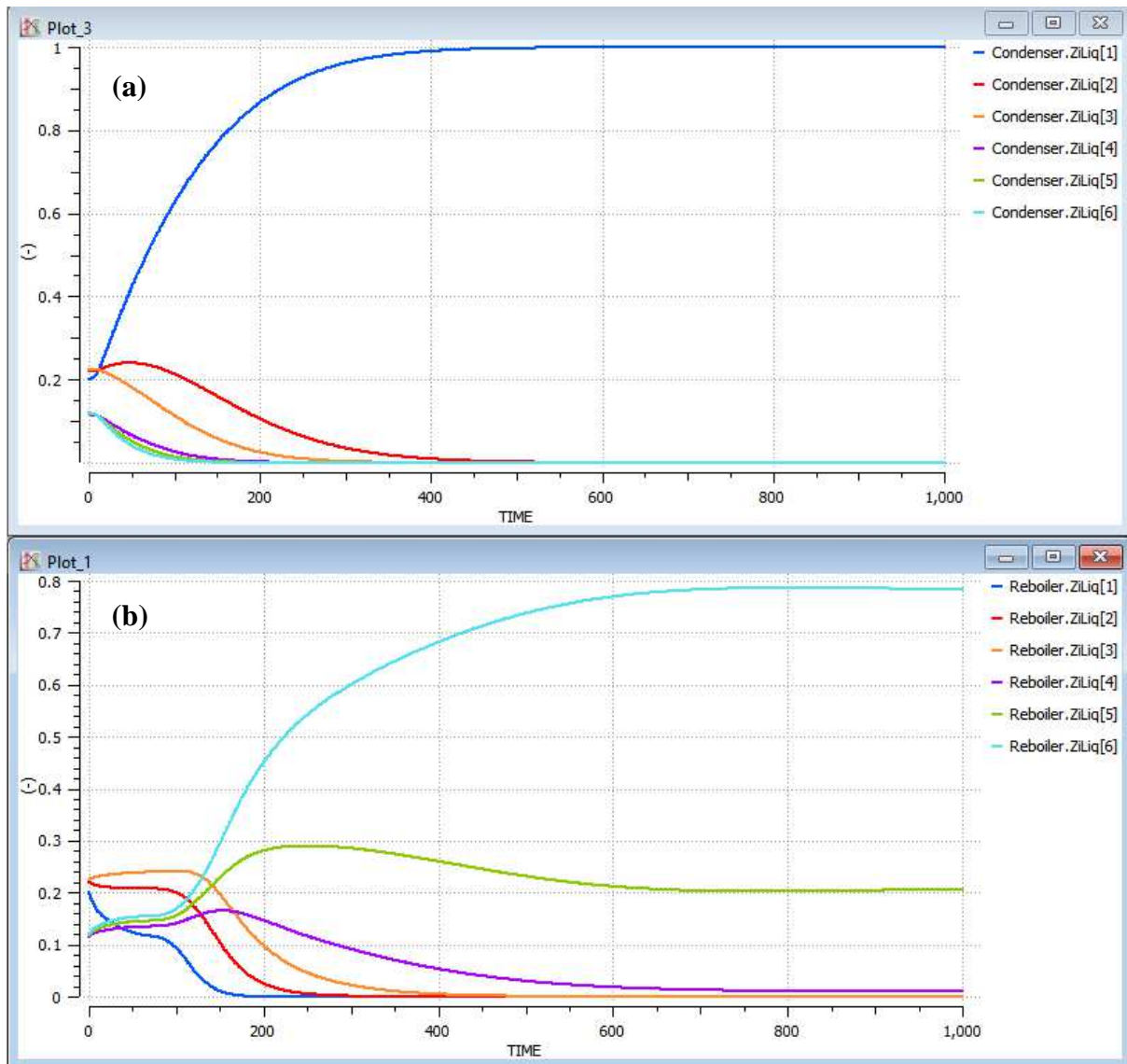
Initial implementation of a distillation column with EcosimPro –KBC Multiflash connection and the hydrocarbon system revealed extremely poor performance that did not significantly improve as the column after difficult initial transient approached the steady state (see Figure 1a). Solver clearly was stumbling and finite difference Jacobians of the ODE system were reevaluated several times at one step. Detailed analysis of the causes was done in Matlab environment to which a special version of our connection library was created. Matlab ode15s solver has all its source code in very friendly environment of Matlab editor-debugger. It was found that many elements in the Jacobian are evaluated incorrectly and this was traced to too small finite differencing steps done in its evaluation by forward finite differencing. At least  $1e-6$  steps in the amount of each substance of a tray were needed for correct finite difference evaluation of the Jacobian. The developers of EcosimPro were asked to provide some user control over the step taken in some variables, in particular the state variables of the UV flash formulation – internal energy and molar amounts. Authors express deep

gratitude to Pedro Cobas Herrero and Fernando Puech Helguero of Empresarios Agrupados for providing this feature of user-control over Jacobian finite differencing step in experimental version 6.1.30 of EcosimPro. At the same time KBC Advanced Technologies improved accuracy of their UV flash algorithm in cases of very small perturbations in input values.

Below are several tests representing progress in the stabilization of the numerical solution. All the tests were done for the first 1000 (s) simulation of a single 110 theoretical tray column with CVODE sparse ODE system solver of EcosimPro at relative and absolute tolerances  $1e-5$  and maximum time step 1.0 (s). Such a test combining a difficult initial transient and easier and slower composition dynamics is representative of real transient simulation scenarios.

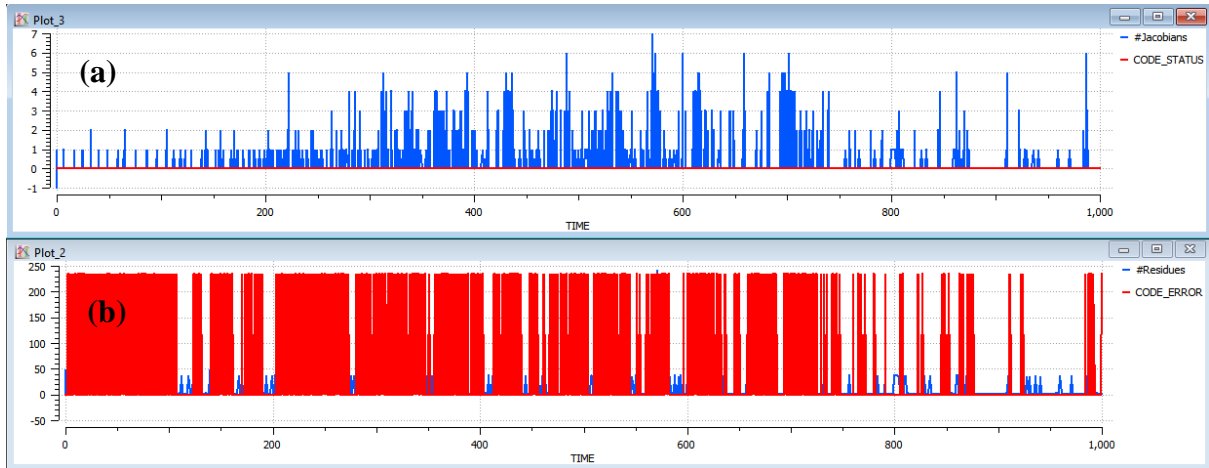


**Figure 3. Cryogenic hydrogen isotopologues system. Plot (a) time evolution of pressure on several trays in the column Plot (b) liquid volume fraction on several trays in the column.**

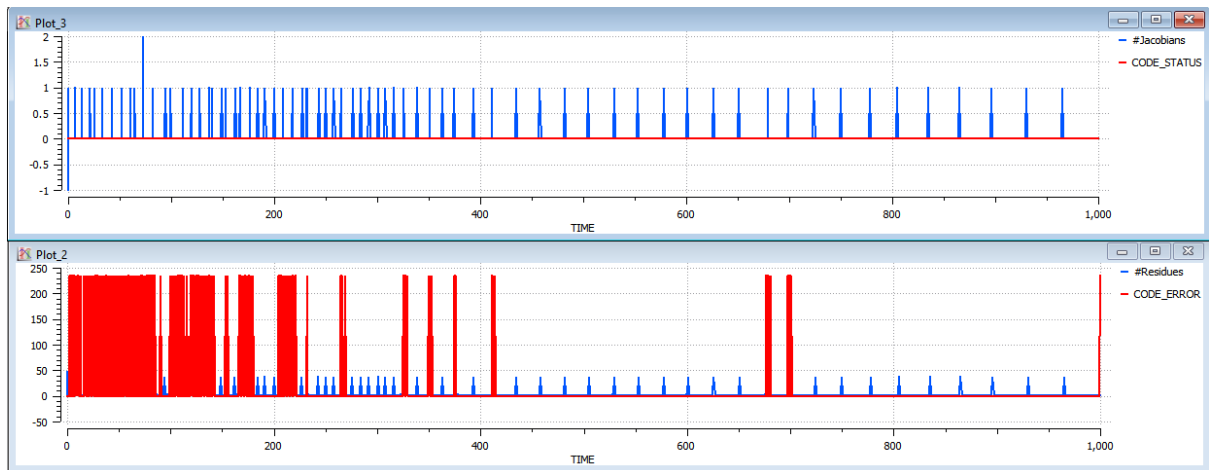


**Figure 4.** Cryogenic hydrogen isotopologues system. Plot (a) time evolution of liquid composition in the condenser (components: 1-HH, 2-HD, 3-HT, 4-DD, 5-DT, 6-TT). Plot (b) time evolution of liquid composition in the reboiler.

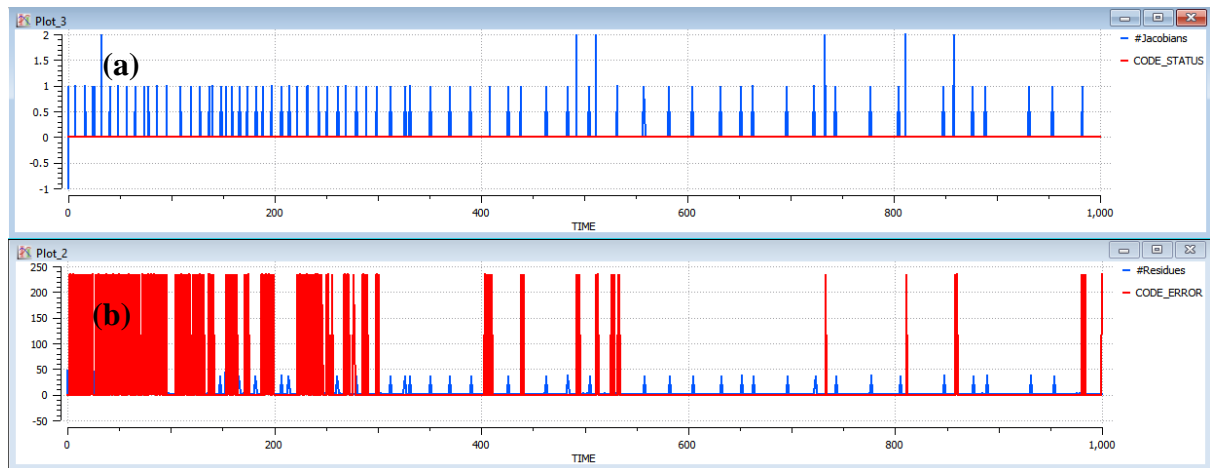




**Figure 5. Initial test with Multiflash 6.2.49 (hydrocarbon system, 2658 (s) of real time). Plot (a) evaluation of Jacobians. Plot (b) integration step contracted (red lines).**



**Figure 6. Test with Multiflash 6.2.49 and EcoimPro Jacobian finite difference step experimental feature activated (hydrocarbon system, 130 (s) of real time). Plot (a) evaluation of Jacobians. Plot (b) integration step contracted (red lines).**



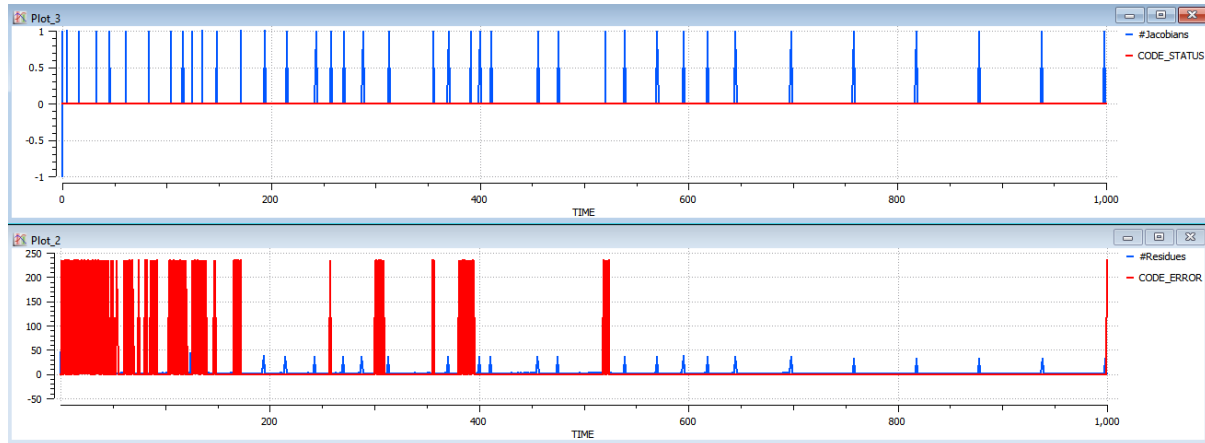
**Figure 7. Test with Multiflash 6.2.55SP1 and without Jacobian finite difference step feature activated (hydrocarbon system, 146 (s) of real time). Plot (a) evaluation of Jacobians. Plot (b) integration step contracted (red lines).**

We can see that both approaches, namely, user-controlled Jacobian evaluation step and tightening of tolerances in the flash calculation produced approximately the same result. Combination of them does not meaningfully improve performance any further. Practically all Jacobian evaluations in both cases were accepted and we see that after 500 (s) reevaluation of Jacobians is repeated. Simulation time for the hydrocarbon system is now an order of magnitude faster than real time that is the minimum requirement for meaningful transient simulation.

Parallelization of UV flash calculations in all the 110 trays was provided with the EcoimPro language feature PARALLEL that relies on OpenMP support of the C++ compiler (Visual C++ 2017 was used). It was very efficient and demonstrated that simulation is clearly bound by calculation of flashes. Speedup of simulation for the test distillation column from 1 core to 16 cores was approximately 15 times.

However for the cryogenic hydrogen system performance is several times slower with the same stable behavior and clear acceleration approaching the steady state as can be seen from the plot below. In

fact number of UV flash calls was at least 20% lower in this scenario in comparison to hydrocarbon tests above (~500 and ~600 thousand UV flash calculations were done in the considered scenarios).



**Figure 8. Test with Multiflash 6.2.60SP1 without Jacobian finite difference step feature activated (hydrogen isotopologues system, 610 (s) of real time). Plot (a) evaluation of Jacobians. Plot (b) integration step contracted (red lines).**

It seems that for the cryogenic system the very narrow temperature span of the components' normal boiling points introduces additional difficulties for flash calculations making them much longer.

## Conclusions and further work

Rigorous UV flash approach to transient modeling of distillation processes was for the first time applied to cryogenic distillation of hydrogen isotopologues. An equation of state based thermodynamic model correctly reproducing both all thermodynamic and transport properties of hydrogen isotopologues and non-ideality of their vapor liquid equilibrium was developed for this purpose. A software link between equation-oriented modeling system EcosimPro and thermodynamic

software KBC Multiflash was developed. Parallelization of thermodynamic calculations was fully implemented in EcosimPro. Speedup of simulation for the test distillation column from 1 core to 16 cores was approximately 15 times. This fact confirms that the availability of massive parallelization can make such a brute force approach as multicomponent UV flash in all volumes at all time steps viable.

It is clear that after the resolution of initially found numerical issues the performance of the UV flash calculation limits the overall performance of the model. KBC Multiflash being a general-purpose thermodynamic software provides very robust and reasonably fast but not the fastest possible UV flash calculations and this is particularly important for the hydrogen isotopologues system at has two phase region at very low temperatures. On the other hand there is nothing that should fundamentally prevent the same level of performance with the cryogenic system. ITER and KBC Advanced Technologies are investigating the possibilities to bring the computational performance of the cryogenic system to the level achieved for the hydrocarbon system.

**DISCLAIMER**

*The views and opinions expressed in this paper do not necessarily reflect those of the ITER Organization.*

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