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# Conclusions from Round Table Discussion during IUT of ESAT 2021 electrolyte thermodynamics challenges - From industrial needs to academic research

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ABSTRACT

Electrolyte thermodynamics is considered one of the most challenging areas of applied thermodynamics. It is an area with a wide range of applications in science and engineering. There are numerous models, both activity coefficient models and equations of state, but despite great successes and achievements of many models for several applications there is little consensus on which are the more generally applicable approaches. There are many controversial aspects, both related to models and to fundamentals. Over many years the Working Party of the Thermodynamics and Transport Properties of the European Federation of Chemical Engineering has organized IUT (Industrial Use of Thermodynamics) workshops in different topics of actual interest. The most recent of these IUTs, 5th in the series, was held (virtually) during the ESAT 2021 conference in Paris. Panellists and participants from both academia and industry attended allowing to include views from a very wide spectrum. This manuscript summarizes the most important points from this workshop in terms of status and needs for electrolyte data and models and concludes with some recommendations for the community, which we hope can accelerate future studies in the field. The target of this work is not to present a general account of successes and shortcomings of electrolyte thermodynamic models, rather it is mostly to focus on the expert views of the IUT participants from industry and academia related to the challenges concerning data, models and applications of electrolyte thermodynamics.

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## 1. Introduction

Many applications in the process industry deal with fluids that contain electrolytic species. While thermodynamic models for neutral molecules are now well established, there are still many unanswered issues related to the presence of ions in a fluid mixture. For this purpose, the Working Party (WP) of the Thermodynamics and Transport Properties of EFCE (European Federation of Chemical Engineering) organized an IUT (Industrial Use of Thermodynamics) workshop that was held during the ESAT 2021 conference in Paris (virtually). The workshop was co-sponsored by the EleTher JIP (Joint Industrial Project).

This was the 5th IUT organized by the WP. The minutes from the four previous IUT workshops have been summarized in various publications [1–4].

Prior to the workshop a panel of representatives from academia, industry and software suppliers with expertise in the area have presented their views. The nine panellists were Nevin Gerek Ince from Aveva, Shu Wang from AspenTech, Gaurav Das from OLI Systems Inc., Olivier Baudouin from ProSim, Christoph Held from TU Dortmund, Laurent Cassayre from CNRS, Georgios M. Kontogeorgis from DTU, Nikos Diamantonis from BP, Susanna Kuitunen from Neste and Antoon ten Kate from Nouryon (Panel Chair).

The panellists were invited to reflect and present their views on the following three open questions:

1. What do you do when confronted with an electrolyte problem?
2. Which modelling approach do you recommend and how do you parameterize, specifically when little or no data are present?

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3. How to create collaboration on an industrially important issue (e.g. electrolytes thermodynamics)?

Following a summary of the comments from the panellists, a two-hour long discussion took place.

There are several reviews in literature about electrolyte models, both on fundamentals and activity coefficient ($G^E$) models [e.g. 5–7] and on electrolyte equations of state, e-EoS [e.g. 8,9]. All these studies are typically written from academia.

The workshop had extensive participation from both academia and industry. This paper summarizes the results from the discussion including but not limited to the views expressed by the panellists. Still, we do not aim to summarize successes and shortcomings of all electrolyte models, but the focus of the discussion is on the information and thoughts during the IUT workshop.

## 2. The needs and problem definition

Needs for data and models relevant to electrolytes are so extensive and diverse that it is absolutely necessary to define the problem as accurately as possible. This problem definition may often be more complex than for non-electrolytes. First of all, it calls for an exact knowledge of **which components** we have in the system (strong electrolytes like salts, weak electrolytes; solvents – water or mixed), **which conditions** (T,P, concentration range/ionic strength) and **which phases** may occur (is there a solid phase or not?), as well as **which properties** are actually needed (only phase equilibrium or also thermal properties; solvent volatilities or ionic activity coefficient for batteries). An important question is whether pH is actually needed to be known/calculated or not. Another valuable question is about the need to have accurate speciation information for a specific problem. These issues are further discussed below.

Moreover, a problem definition in industrial applications will often include expectations about the required accuracy, effort, timing and business case. The actual problem to be solved needs to be specified e.g. prevent electrolyte entering certain flow, prevent or maximize solid formation, choose appropriate materials for equipment, aim to understand laboratory results or design/trouble-shoot full scale process. Or even how electrolytes affect the behaviour of other components in the system and how minority components may cause troubles in operations (e.g. corrosion).

Based on the problem definition, some **assumptions or simplifications** can be made, and expectations can be outlined. The real difficulty is to determine the correct/acceptable level of simplification. In practice, the level may change during the project development, as a gross design may not need as many details as the detailed design. For example, in the case of VLE (depending on temperature and pressure) usually we can assume the presence of only solvent in the gas phase. However, at some point it may become important to have access to the presence of minority compounds in one phase, either because of toxicity or corrosion aspects.

Depending on the phase, salting out will occur or a salt might stabilize a component that is distributed between two liquid phases. SLE can also be problematic since it is usually known only for water which kind of solid will precipitate, yet, the presence of co-solvents heavily determines the solubility limit of the salt, or could even affect the type of salt that is formed. Standard states are particularly important for SLE and such data for the diverse solid forms are difficult to get. Mixed solvents can be tricky and especially the combination of solvent – salt is important as this determines the kind of additional species that might be formed (e.g. ion pairs). This, in turn, will influence dramatically the phase behaviour.

Some of the industrial problems are particularly complex and there is significant lack of **data**. It appears that about 90% of all studies relate to data at ambient conditions and for systems comprising (pure) water. Often, such knowledge cannot be simply transferred to other temperatures or pressures, e.g. due to the complexity in solution enthalpy effects. Hence, understanding trends from available data both from literature and from proprietary experiments is very useful and this is a common practice in industry, even if such data are from "similar" systems and not exactly from the systems of interest. In some cases, pH and pKa data can be particularly useful and may be not very difficult to measure. Nevertheless, it has been stated that for electrolytes, unlike more conventional systems, the knowledge about the subsystems does not necessarily lead to a satisfactory representation. This is because new components can be formed that do not occur in the subsystems (e.g. sour gases, well known aqueous mixtures, with $CO_2$ and $NH_3$ which can react and form non-volatile components, increasing the solubility of these gases).

## 3. Which models can be used for electrolyte solutions?

### 3.1. Theory

To accurately model a multicomponent electrolyte system, interactions (such as long-range electrostatic, short-range dispersive) between different ionic and neutral solution species need to be explicitly defined at the theoretical level. This was recognized in the workshop.

Still, theoretical developments were discussed only very briefly in the workshop and most of the approaches use some form of Debye-Hückel or MSA (Mean-Spherical Approximation) theories, the latter mostly in e-EoS. Differences between the two approaches when combined in general electrolyte models appear to be small and there is no consensus yet whether the concentration dependency of relative permittivity is important and must be included in the modelling. Several participants commented on the importance of the Born term in both e-EoS and electrolyte-$G^E$ models, especially for LLE and mixed solvents. The Born model was debated and some expressed the view that the term, while useful, is too simplistic (lack of entropic contribution, very weak pressure effect, temperature effect only via the relative permittivity, etc.). Moreover, whether the advanced models like non-primitive MSA can capture qualitative trends was briefly discussed without definite conclusions.

Finally, it was mentioned that for estimating the properties of systems for which little experimental information is available, a corresponding-states approach is promising. In pure ionic fluids, corresponding-states methods have been proven useful for estimating the properties of salts at high temperatures. However, no rigorous corresponding-states treatment is available for salt–water mixtures. At the same time, analysis of the phase behaviour of several electrolyte systems reveals significant regularities, which may be regarded as a manifestation of a corresponding-states behaviour.

### 3.2. Excess-Gibbs energy models and electrolyte equations of state

As expected, the choice of the modelling approach to use will depend on the application of interest (VLE, LLE, SLE, other properties) but also on the availability of model parameters for the applications of interest and especially the familiarity with the specific approach and availability in commercial software. The (non-)availability of model parameters is of some relevance for commercial models, although there is the option in many of these commercial models to fit the parameters if experimental data are available.

For all these reasons, activity coefficients ($G^E$-approaches) are by far the ones most often used in practice as they are the only ones available in most software tools.

In general terms, among those $G^E$ models, the model which has been mentioned by many in the discussion was electrolyte NRTL (eNRTL), possibly due to its availability in several simulators and software packages (Aspen Plus, AVEVA, Simulis Thermodynamics). It requires a lot of experimental data for the estimation of parameters (see discussion in next section) and often these data are not available for specific applications. Yet, it is designed to be applicable to both aqueous and mixed solvent systems.

Other models have been mentioned as well esp. Pitzer, extended UNIQUAC, SIT and the Mixed Solvent Electrolyte (MSE) model by OLI. For very special applications, some specific models were cited like Engels for mixtures with strong acids (e.g. a mixture of sulfuric and nitric acids), or the Helgeson-Kirkham-Flowers (HKF) which can be used to compute chemical equilibrium constants, liquid molar volume, enthalpies, etc. from pure true species properties. Some of the aforementioned models are ion-specific and some are salt-specific but comparisons between the models have not been mentioned during the workshop, not even for a limited number of systems. In the authors' view, there are only few comparisons between electrolyte models carried out on equal terms.

There are many considerations of importance related to thermodynamic models for electrolytes, and while connected, the following rather independent aspects can be mentioned, and the points below apply to many/most of the literature approaches:

1. Models - although they can be to some extent equivalent when they are targeting the same property (e. g. activity coefficient or fugacity coefficient) – they do not perform equally, partially because their theoretical foundations are different.
2. Industrial use relies either on commercial/publicly available models or on in-house models.
3. External models can sometimes pose problems in regards to refitting parameters. So even if data are available, it is difficult to use the data to improve the models. Nevertheless, commercial software tools typically provide a possibility to regress parameters to data, yet the regression tools may be cumbersome and challenging, esp. for electrolyte systems.
4. Electrolyte models are complex and require special algorithms to assure cost-effective convergence. It is costly and elaborate to implement such models (for commercial software vendors as well as for in-house models) in particular if these model frameworks are general purpose built.
5. Electrolyte models need plenty of parameters, but experimental data are fragmentary or missing. Moreover, in these models the parameters appear to have a high level of correlation and dedicated direct measurements to quantify parameters appear difficult.
6. If data are missing, there is a lack of proper correlation methods to estimate the parameters.

Another major issue is the need to achieve consistency between the selection of the true or model-intrinsic components, the relevant reactions to be considered, the data for the model fitting that can usually not be measured ion-specific, and the required mapping of the model species to the useful apparent components for engineering purpose.

Electrolyte equations of state, based on SAFT or cubic equations of state (with/without association), have been discussed only very briefly, possibly due to the fact that these models are under continuous development and are not available in commercial software tools. Still, it has been mentioned that various versions of e-SAFT e.g. group-contribution versions of PC-SAFT or the electrolyte CPA are expected to play a significant role in the coming years. They require fewer parameters than electrolyte Gibbs excess models, but today they are not used as often as the activity coefficient models in practice. Interestingly, there has been very little discussion about properties which can only be predicted by e-EoS e.g. densities at high pressures.

When searching for a predictive approach, it has been mentioned that at least in one software tool (Simulis Thermodynamics) a predictive Gibbs excess model based on modified UNIFAC is available (the ULDPS model). This model has specific groups for ions, that take into account short-range interactions, while a Pitzer-Debye-Hückel term is used for long-range interactions, and which also takes into account species solvation. Interestingly no/very few publications of this approach exist and there are no comparative validations against the other popular $G^E$ models mentioned above. This model is not well-known as it has not been known by the majority of the participants who expressed actually the interest for a predictive electrolyte model.

Finally, it was mentioned that COSMO-RS methods could contribute in the case where little or no experimental data are available and some recent promising works have been cited but these studies are at an early stage.

The number of modelling approaches is rather overwhelming and despite some preferences, several of the industrial participants expressed an interest for a decision tree or similar form for assisting in the choice of a suitable model for a specific case. We feel this is not easy and it may depend on opinions and traditions, as we outline in the forthcoming section.

### *3.3. Suitable models depending on properties and conditions*

While the discussion in the previous section is a general presentation of the main conclusions from the discussion, it was also emphasized quite emphatically that different applications may need different approaches, as there is clearly no unique solution to all problems. Following guidelines have been discussed:

1. **Phases present**. In case of VLE (depending on temperature and pressure) usually we can assume the presence of only solvents and other related compounds in the gas phase (but not of the electrolytes) and the use of models without the Born term should work fine with versions of eNRTL, Pitzer, and some electrolyte equations of state. On the other hand, LLE is more difficult as ions will distribute between two phases and models with the Born term may be required, although there is no consensus on this.
   Correlative models such as eNRTL work if the parameters between ions and second solvent are available. Default parameters are available, but those do not turn out to give the desired results in all cases. On the other hand, SLE is problematic and the results are very sensitive to the solid properties; changing them by 1% can significantly change the modelling results. Additionally, the kind of solid must be known prior to modelling SLE. In the literature there are data for aqueous solutions, but the problem becomes very delicate for mixed solvents.
2. **Solvents.** Especially the combination of solvent – salt is important as this determines the kind of additional species that might be formed (e.g., ion pairs). If the solvent is only water, most models work well, but many models are, however, only parameterized for a limited number of salts. If a co-solvent is present or the solvent is water free, then a very good model is required and usually new experimental data are required to validate the accuracy of model predictions.
3. **Data availability.** A lot of data is available for standard salts like alkali halides. However, other salts such as those acting as base in chemical industries are less studied, and more simplifications might be required. One such assumption is often the complete dissociation of the salt, which is justified using ion-specific approaches. It was mentioned by some participants that, in general, ion-specific approaches are to be preferred and that these

models are more powerful and physically more reasonable, as they also have fewer parameters and can extrapolate more reliably also in the case of rather few data. Again, there is no consensus, and please notice that eNRTL is a salt-specific model. A full section is devoted to data and databases, see below.

4. **Conditions.** The modelling of aqueous solutions at ambient and non-extreme conditions is quite well-understood, yet the modelling of mixed solvents and/or extreme conditions such as high concentrations and high temperatures are far more challenging. For such conditions, temperature-dependent model parameters may be required as the behaviour of electrolytes with temperature is non-linear. Using models that are not validated to higher temperature and pressure is not recommended and validation through temperature (and pressure-) dependent LLE, SLE or VLE is required. Predictive approaches may not always be successful but they may be useful at extreme conditions where little or no data are present and at high concentrations / high temperature where ion pairing occurs and dielectric constant is decreased.
5. **Simplicity vs. complexity.** This has been discussed extensively and several industrial colleagues stated the importance to find the correct balance in modelling, avoiding too complex models when not needed e.g. in the preliminary design stage and increasing the complexity in the detailed design phase. There are at least two types of complexity in this context:

- complexity by the kind and number of properties needed for the purpose (Basic design: phase equilbrium, enthalpic properties, density; Detailed design: additional transport properties, surface tension, diffusion coefficient) and
- complexity by higher model accuracy (especially if different accuracy is needed for some properties, e.g. water saturation of the vapour), more detailed component specification or better extrapolation ability.

  In some cases, only bulk properties are needed; in others, partial molar properties (e.g. activity coefficients). In this latter case, sometimes minority components (impurities) may be required, thus increasing the complexity of the problem. As example, if volatility of neutral species is required, the knowledge of ionic strength may be sufficient; on the other extreme, if toxicity in living beings is searched, the activity of minority compounds may be crucial! Further, if no data are available, the use of the best models is recommended that has shown good predictive power for similar systems as the system under study. The model is used for guiding purposes in these cases and validation by experiments is required.

In the case of weak electrolytes, sometimes their electrolyte character can be neglected (e.g. formic or acetic acids, even $SO_2$, $NH_3$, $CO_2$ and $H_2S$ depending on the application domain the model is used for, i.e. do we need to calculate pH, to know the true composition of the mixture and so on). In some cases, the assumptions can be crude but still usable e.g. when dedicated models available for some specific applications (e.g. the Soreide-Whitson model for sea water and hydrocarbons mixtures). But care should be exercised, and no generalisations can be made. The actual choice will depend on the problem to be solved. It is sometimes convenient in practice to treat a complex electrolyte solution as NaCl-analogue. But to use NaCl as analogue for describing the behaviour of other solutions will in many places significantly falsify results, for example in biological systems (e.g., the role of $Mg^{2+}$ in molar concentrations on metabolic reactions).

## 4. Databases and model parameter estimation

The databases and the parameter estimation of electrolyte models were topics heavily debated in the workshop. On one hand, there is satisfaction about the availability of many databases that several of the participants have access to, e.g. Detherm, LLNL, Thermoddem, NIST, ThermoXL, Thermochimie, PhreeScale, FactSage (for solid compounds), ProPhyPlus (for pressure application requiring an EOS for the vapour phase), and others, including the REAKTORO or JESS frameworks for chemically reactive systems. The literature on databases is indeed extensive. There were, however, some complaints concerning the lack of open and easily accessible data sources. In response, other companies expressed the view that maybe the available commercial databases are actually sufficient but more structured databases are needed, with the data also available in digital form.

Several industrial participants mentioned that measurements are sometimes carried out for new systems for which there is a lack of data e.g. water activities, freezing points and solubility. Nonetheless, it was not clear whether such data were being published. Considering competitive advantage, there is a natural tendency for industry to keep the data private.

Overall, there was a feeling that the literature in the field of electrolytes is rich, both at the experimental level and in the models implemented for some systems. Often the first thing to do is to look at what has already been studied in the area of interest. Nonetheless, given the huge variety of systems and conditions, next to the lack of proper extrapolation and prediction methods, there is still ample room and need for further exploration.

The reason why databases and experimental data were such a “hot topic” is that there is a broad consensus amongst participants that for all typical electrolyte models, a large number of adjustable parameters are required. There was a general feeling that electrolyte models seem to require a lot of parameters which are often difficult to properly regress. These must be fitted and validated using various types of experimental data, including vapour-liquid equilibria, osmotic and activity coefficients in completely dissociated aqueous systems, solubility of solid salts in water, organic solvents and mixed solvents, densities, heats of mixing and dilution, heat capacities and various speciation-related data (pH, acid dissociation constant as a function of solvent composition) as well as Gibbs energy of transfer of electrolytes. Another issue is that some models cannot be fitted to a unique model parameter set (depends on the amount of data) and we observe that many parameter sets can satisfy the fitted data.

Such a multi-property approach can allow to accurately capture the phase behaviour, thermodynamic and caloric properties of the complex multicomponent electrolyte systems. Furthermore, a comprehensive thermodynamic modelling approach often demonstrates excellent predictive ability, which is desirable as in certain solution conditions no experimental data exist.

It was often mentioned that in many cases new parameterizations of published and commercially available models are needed. For this, the regression tools available in simulators can be used e.g. in PHREEQC or the OLI regression tool for the MSE model or electrolyte NRTL in Aspen Plus. Some mentioned that the availability of a model’s parameters based on high quality data can be more important than the actual model functionality in some practical applications.

### 4.1. Concerns and recommendations

There have been several concerns related to the interplay of experimental data and regression needs of electrolyte thermodynamic models:

- Contrary to non-electrolyte models, there is a concern whether parameterization of a lower-component subsystem provides good prediction of the multi-component system, particularly due to the chemical effects.

- Algorithms were extensively discussed and there can be additional challenges in case of electrolyte modelling especially for reactive systems – speciation – involvement of reactions such as for weak electrolytes.
- The question was raised on whether data sciences can be used to "fill the gaps", and whether they can be useful in model development and validation.

The model validation after the parameterization is an area of particular concern. Can we assess whether the results can be expected to be qualitative or quantitative? Is the model optimistic or pessimistic from the study point of view? How to ensure that the design is on the safe side if there are uncertainties in the simulation model? Can we assess the impact of this uncertainty on the design? Also, taking into account the general shortcoming of steady-state flowsheet simulation, as in reality, phases are not necessarily in equilibrium. Several participants recommended to perform a sensitivity analysis of the model at the expected conditions and to consider, if possible, the uncertainties involved in the parameter estimation. Such sensitivity analyses are particularly important as there are often many model parameters and it is not easy to assess their relative weight or importance. It has also been recommended, in case of very few data for the actual systems of interest, to look for data and perform validations for systems with "similar compounds" and adapt the degree of parameterization (number and type of parameters) depending on the quantity and type of available data. This may, of course, be considered an indirect way to estimate parameters through a constraining approach.

## 5. Discussion – comparison to EFCE survey and summary of workshop papers of IUT

Recently the WP of Thermodynamics and Transport Properties of EFCE carried out a survey on industrial needs for such properties. 37 companies answered and the results have been recently published [10]. Electrolytes were a hot topic and it may be relevant to compare the findings of this survey with those from the recent workshop. In the text below we summarize the survey results for electrolytes so that the interested reader can compare with the workshop results presented in the previous sections.

According to the survey results, a large number of companies agreed that modelling of electrolyte systems remains a major challenge, both from a fundamental point of view and from a more "practical" point of view (e.g. many parameters not available for important systems in e-NRTL).

It has been extensively stated in the survey that electrolytes are present in many processes, including bioprocessing, but that the electrolyte models are more complex than the non-electrolyte ones, and much more difficult to use for practicing chemical engineers. Lack of standardization has also been mentioned as a problem when it comes to using these models, even for the most established models like e-NRTL. Many companies urged for a critical review/comparison/evaluation of these models, like what has been done for non-electrolytic (predictive) models.

There have been very few suggestions provided on what to do/which models to use to address these significant challenges, but several companies (which use Aspen Plus and maybe also other simulators) discuss extensively e-NRTL, a model often used but with serious limitations, e.g. a clear methodology to fit parameters is required. In addition, many companies emphasize that e-NRTL parameters may be missing in the database for specific systems of interest to some applications e.g. radioactive and toxic compounds.

Despite the lack of much discussion on alternatives, the companies in the survey stated that improved and increasingly predictive models are required for electrolyte solutions, with limited need for adjustable parameters and data regressions. The predictive capabilities should include high concentrations, and speciation behaviour; both areas where significant improvements are needed. Many companies expressed concerns about most existing models requiring large datasets or having no predictive power outside the experimental range (in particular the difficulty to predict multicomponent systems from lower order systems, like ternaries from binaries).

The survey included very few comments on equations of state for electrolytes e.g. those based on SAFT, since they are not available in (most) commercial simulators. A single company noticed that there have been some positive developments, such as the inclusion of Coulombic interaction terms in SAFT, while another company mentioned that the development of models (GC PPC-SAFT) that could be used in Aspen Plus would be a major improvement. Not everybody is fully satisfied with e-NRTL and some mention that testing electrolyte SAFT models should be given more consideration.

The authors of the survey manuscript concluded that electrolyte thermodynamics is an area where development of new models require advancement of fundamentals e.g. the role and importance of the Born term; the description of ion-solvent interactions; the role of individual ion activity coefficients (even if they are not entirely accepted by the community) and more. Finally, the electrolyte part of the survey was ended with this comment by the authors of the survey:

"We hope that in the future we will see "pragmatic" developments of electrolyte models with both the classical approach of activity coefficient models (like e-NRTL, extended UNIQUAC and Pitzer) and the advanced e-EoS and we believe that this will provide to industry a larger flavour of potentially successful electrolyte models."

Finally, it is interesting to note that the need for better/more accurate electrolyte thermodynamics had been expressed also in the previous survey from the working party published 10 years earlier [11].

## 6. Collaboration and recommendations to the community

The collaboration opportunities have been extensively discussed within the area of electrolyte thermodynamics and there is a general consensus that it is important to create common ground for exchange of information between industrial and academic experts as well as software providers. There is quite some diversification in the field with many research teams having own tools and databases, but this should not prohibit discussion on how some consolidation can be achieved.

Joint Industrial Projects (JIP) is one way to have such a way of working and the Elether JIP [12] is mentioned by many as an exemplary and successful initiative. The creation of consortia like those already existing for pure components databases (DIPPR from AIChE) or group contribution predictive models (UNIFAC Consortium) is also an interesting track that creates a synergy on the long term, with clearly established development axes by the different members of these consortia. A careful preparation prior to the creation of these JIP is however emphasized. Well-defined targets will facilitate to bring the case to decision-makers. In addition, the findings should be implemented in some commercial simulation tools (which modelling approach is the best, best practices in parameter regression etc.). The role of software vendors is, thus, quite relevant in this context.

Some examples of interesting targets for such collaboration have been mentioned:

1. To develop or agree upon a small number of benchmark cases/challenges which could allow discussions without confidentiality complications.
2. To develop a "standard" database for model development and/or model validation, as recently proposed for non-electrolytes by Jaubert and co-workers [13]. A consolidation – combination of available electrolyte databases would be a useful, albeit difficult task. Of course, such a "standard" database will still be simply used as guidance as the range of relevant systems for electrolyte applications is very extensive.
3. To stress and prove the importance of electrolytes to current technology, including a wider range of applications (Power-to-X, batteries, etc.) and climate challenges in a way that is easy to demonstrate to policy makers and management levels.
4. To create a network of laboratories with special expertise in experimental methods - measurements relevant to electrolytes.
5. To develop a common tool for optimisation, calculation with various models, with the same format for all experimental data (that could be shared) would probably enhance further collaborations on these topics and the investigation of the use of open-access platforms is recommended. This may require a change of paradigm by some stakeholders, but it is worth investigating. The open source paradigm, which is working in other fields, may be also considered here.
6. Despite the low success rate of such applications, EU and national calls for funding can be pursued, as the industrial participation is required in several of them nowadays.

Finally, it has been often mentioned that the link to actual "customer-industry" problems/case studies should be particularly stressed and can define the scope of a collaboration. Although, it was mentioned that there are various modelling tools, there is no consensus about the strengths and weaknesses of the various thermodynamic models. A collaboration between academia, industry and software providers (consultancy firms) can be very beneficial as new challenging processes appear with the need to have more predictive methods, typically related to the circular economy.

## 7. Conclusions

The IUT symposia have been established to promote synergy between industrial needs and academic research [1–4]. In each of these symposia, a round table discussion has been held where different stakeholders were invited to present their view of the coming challenges. The 5th IUT symposium, held virtually during the ESAT 2021 conference, focused on electrolyte thermodynamics, which was also identified by the survey paper [10] as being one of the major challenges in the area of chemical engineering thermodynamics. The discussion has brought up several interesting topics:

- The close interrelationship between the problem definition and the degree of complexity of the modelling approach,
- The limitations of the (very few) models that exist today in commercial simulators, and specifically their lack of predictive capacity which is a result of the large number of adjustable parameters,
- The large consensus among the participants that collaborative efforts are needed to address the new challenges that will come up because of the complexity of the systems that address current world's grand challenges (e.g. as laid down in the Sustainable Development Goals (UN-SDG's)), like circular economy and energy transition.

## Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

## CRediT authorship contribution statement

**Georgios M. Kontogeorgis:** Conceptualization, Methodology, Writing – original draft. **Antoon ten Kate:** Conceptualization, Methodology, Writing – review & editing. **Martha Hajiw-Riberaud:** Conceptualization, Methodology, Writing – review & editing. **Jean-Charles de Hemptinne:** Conceptualization, Methodology, Writing – review & editing.

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