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ORIGINAL RESEARCH ARTICLE

# Process modelling and thermodynamic analysis of cyanuric acid vinylation with acetylene

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## ABSTRACT

The vinylation of cyanuric acid derivatives with acetylene provides an industrially useful method for making trivinyl-substituted heterocyclic compounds; however, there has been little process-level research on this reaction system in the open literature. Therefore, this work fills that knowledge gap by evaluating the vinylation process through a combined stoichiometric, thermodynamic, and Phase Equilibrium investigation using the Aspen Plus steady-state model. The process consists of three sub-phases: (i) A feed mixing stage, (ii) an RSTOIC reactor running continuously at 90 °C and 1.52 bar, and (iii) a downstream flash separation unit. The Non-Random Two-Liquid (NRTL) activity coefficient model and the ideal gas assumption were used to capture liquid-phase non-ideal behaviour and vapour-liquid equilibrium. All thermophysical properties of the target trivinyl product ($C_9H_9N_3O_3$) were estimated using the group contribution method, yielding an average error of no more than 1.73%, confirming that the model is appropriate and reliable for engineering-scale applications. The suggested processing layout exhibits very good conversion capability, conforms to the laws of thermodynamics, and is grounded in an accurate theoretical framework to support an initial process design. This work is intended as a preliminary, equilibrium-based screening framework rather than a kinetically validated design tool; it provides a reliable simulation basis for reactions in this class and, as such, offers a quantitative foundation for future research. Future work should include a thorough kinetic model and experimental confirmation to evaluate industrial scale-up potential rigorously.

***Keywords:*** cyanuric acid; vinylation; aspen plus; vapor-liquid equilibrium; thermodynamic analysis

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## 1. Introduction

The cyanuric acid family of compounds is now considered a highly promising class of starting materials for designing superior materials due to (i) their very high thermal stability, (ii) inherent chemical inertness, and (iii) availability of nitrogen functional groups for specific chemical modification. Recent developments in the chemistry and uses of cyanuric acid-based materials indicate the growing demand for high-end materials for applications such as thermal management, reinforcement, and catalysis. This has led to a

keen interest in the discovery of innovative applications of cyanuric acid-based materials, as well as novel chemical modifications of cyanuric acid materials[1-5].

The modification of heterocyclic systems using acetylenic vinylating agents is a highly strategic reaction in this field of chemistry. Many new reactions based on the usage of acetylenic vinylating agents have recently been devised. The introduction of a vinyl group into nitrogen enables further reactions, including the polymer's participation in radical polymerisation and crosslinking. This gives rise to various polymerisable materials derived from stable, unreactive substances; therefore, a whole new field of research emerges[6]. Nitrogen vinylation involves nucleophilic addition in a basic medium (potassium hydroxide in dimethyl sulfoxide, KOH/DMSO). Under such conditions, the reaction proceeds in steps, in which vinyl moieties add to nitrogen centres (or vinyl centres), ultimately producing mono-, di-, and tri(vinyl) substitutions on the same molecule[7]. While the mechanism underlying such a process is known at the molecular level, translating it into a quantitative description that accounts for gas-liquid phase relationships and the non-idealities of the polar solvent remains an open engineering problem due to the many interacting parameters involved. Very few process-level studies of this reaction family exist[8-10], and, to the best of our knowledge, none report an Aspen Plus (or equivalent flowsheet-simulator) treatment of cyanuric acid vinylation specifically; the studies most closely related in synthetic scope (refs.[6,7] on N-heteroarene and alcohol/thiol/nitrogen vinylation, and ref.[12] on multicomponent-reaction selectivity) are laboratory mechanistic and selectivity studies and do not include stoichiometric, VLE, or thermophysical-property simulation of the reaction system.

According to the literature, studies on this group of reactions have contributed, in an unbalanced yet significant manner, to the methods used in this field of research. Most scientific work on this group focuses on their mechanisms and products from a synthesis perspective, with limitations in transformation, selectivity, and the structures of isolated compounds[11,12]. More specifically, four complementary gaps can be identified in the existing literature: (i) the absence of reaction-kinetic data for the stepwise vinylation of cyanuric acid; (ii) the lack of experimental vapor-liquid equilibrium (VLE) measurements for the DMSO–acetylene–cyanurate system; (iii) the absence of process-flow (flowsheet) simulations describing mass/energy balances and phase behaviour for the reaction train; and (iv) the lack of thermophysical property data or predictions for the trivinyl cyanuric acid product. The lack of this integrated approach is not purely a theoretical shortcoming: establishing a validated stoichiometric–thermodynamic–VLE modelling framework is of direct practical value because it supplies the mass and energy balances, phase-distribution data, and preliminary sizing information that are prerequisites for reactor and separator design, solvent/catalyst screening, and scale-up assessment, independently of whether detailed kinetic data are yet available[13,14].

The simulation of chemical reactions using software such as Aspen Plus has been validated to create a computational framework that will provide solutions to the two problems stated above. In the case of non-ideal behaviour of liquid phases resulting from the use of DMSO as a solvent, NRTL is the conventional choice to describe the activity coefficients of the system for such polar organic mixtures; the implications of this choice for the present, KOH-containing system are discussed explicitly in Section 2.1 and in the Limitations subsection. On the other hand, the vapour phase can be modelled using an ideal-gas equation of state even at moderate pressures. By combining descriptions of the physical properties and the reactor stoichiometry, more information can be obtained than from experiments alone[15,16]. The Aspen-based VLE/absorption modelling methodology used here follows precedents established for other industrially relevant, strongly non-ideal liquid systems, including ionic-liquid process simulation and e-NRTL-based modelling of high-concentration amine solutions. Cyanuric-acid derivatives are themselves of established industrial relevance, e.g., in ammonia–cyanuric acid co-production for boiler denitrification, which motivates a rigorous process-simulation treatment of their vinylation chemistry as well[17-19].

The present research project bridges a current knowledge gap by modelling the vinylation of cyanuric acid using the Aspen Plus platform. This project merges the analysis of four distinct categories of data:

stoichiometry, thermodynamic consistency, VLE behaviour, and thermophysical property prediction, all in a single reaction process, a combination which has not been attempted previously for the same reaction scheme. The objectives of the current project include: (i) quantitative evaluation of process efficiency using mass and energy balances; (ii) phase characterisation for each process step in the entire reaction; (iii) determination of the VLE and volatilities of all the process compounds; and (iv) thermophysical property validation of the final computed/simulated trivinyl compound ($C_9H_9N_3O_3$).

# 2. Materials and methods

## 2.1. Reaction system and physicochemical model

The reaction studied is the base-catalysed nucleophilic vinylation of cyanuric acid ($C_3H_3N_3O_3$) with acetylene ($C_2H_2$) in a dimethyl sulfoxide (DMSO) solution, using potassium hydroxide (KOH) as a homogeneous base catalyst, the classical KOH/DMSO "superbase" system used for N-vinylation of N–H–acidic heterocycles. Mechanistically, the nitrogen-bound hydrogens of cyanuric acid are deprotonated by KOH/DMSO, and the resulting nitrogen anion adds across the acetylene triple bond, generating mono-, di-, and finally tri-vinyl-substituted product in a stepwise addition sequence. In the absence of measured rate constants for the intermediate mono- and di-vinyl species, the two intermediate addition steps are lumped together with the final step and represented by a single overall stoichiometric reaction (R1):

$$C_3H_3N_3O_3 + 3C_2H_2 \rightarrow C_9H_9N_3O_3 \quad (R1)$$

This lumping is an explicit simplification: intermediate mono- and di-vinyl species and any side reactions are not tracked individually, and only the net (fully vinylated) transformation is quantified. This restriction is revisited in the Limitations subsection.

Cyanuric acid was chosen as the limiting reagent, and a target conversion of 80% was specified for the RSTOIC block. Both the target conversion (80%) and the reactor operating point (90 ℃, 1.52 bar) were selected to correspond to the conditions reported for the experimental, laboratory-scale KOH/DMSO-catalysed vinylation of cyanuric acid with acetylene under homogeneous catalytic conditions, so that the process simulation reproduces a realistic, experimentally anchored operating regime rather than an arbitrary one as per the characteristics of a strongly polar medium such as the DMSO system, the Non-Random Two-Liquid (NRTL) activity-coefficient model was used to account for liquid-mixture non-ideality. At the same time, the vapour mixture is treated as an ideal gas. Default (Aspen Plus built-in) NRTL binary interaction parameters were used, since no experimentally regressed parameter set exists in the literature for this specific DMSO–acetylene–cyanurate–KOH system; this is acknowledged as a source of quantitative uncertainty in the predicted K-values (see Limitations). Furthermore, because KOH is present only in a small, sub-stoichiometric amount relative to DMSO (0.1 vs 15 $kmol \cdot h^{-1}$, i.e. below 0.6 mol%) and is treated here as a homogeneous catalyst rather than as a fully dissociated electrolyte species, the conventional molecular NRTL model was used instead of the electrolyte-specific ELECNRTL model. This is a deliberate simplification appropriate for a preliminary screening study. Still, it neglects activity-coefficient corrections arising from electrolyte dissociation and is explicitly flagged as a modelling limitation rather than a validated representation of the salt-containing liquid phase. Thermophysical properties of the desired product ($C_9H_9N_3O_3$) were predicted using the Joback group-contribution method, chosen because it is the default Aspen Plus group-contribution method and requires only the molecular structure as input, which is appropriate at this preliminary process-screening stage. It is noted that the Joback method is known to yield larger deviations for small molecules, and that improved group-contribution methods (e.g., Marrero–Gani or Ambrose) could reduce the estimation error for a molecule of this size; adopting these methods is identified as a refinement for future work rather than implemented here, since it would require re-parameterising the Aspen property system beyond the scope of the present preliminary study, and DIPPR group-contribution approaches of Aspen Plus, with the associated

mean absolute error (MAE) computed by Aspen Plus Property Estimation by benchmarking the group-contribution predictions against the measured property values held in Aspen's internal DIPPR databank for structurally related compounds (Aspen Plus's standard property-estimation validation procedure); no independent external experimental data set for the specific trivinyl cyanurate product was available for benchmarking, which is acknowledged as a limitation.

## 2.2. Process configuration and simulation basis

Cyanuric acid and DMSO are introduced in large amounts into the first mixing vessel in each stage of the process, together with the KOH catalyst (feed stream FEED1); a second feed stream (FEED2) supplies pure acetylene as the vinylation reagent. The process is simulated in three continuous, steady-state stages (**Figure 1**): (i) a feed-mixing stage (MIXER block), (ii) a continuous stoichiometric reactor (RSTOIC block), and (iii) a downstream two-phase flash separator (FLASH2 block).

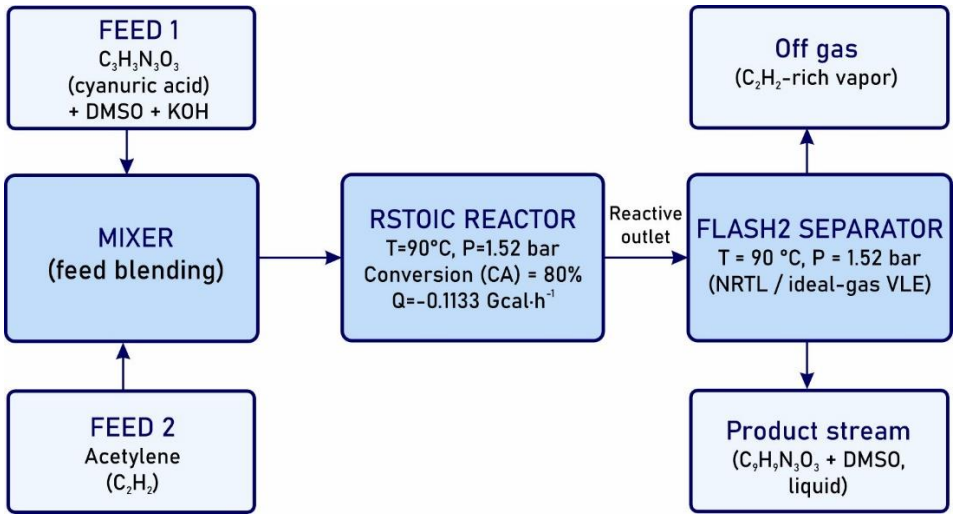


**Figure 1.** Aspen Plus process-flow schematic of the cyanuric acid vinylation process (feed mixing → RSTOIC reactor → FLASH2 separator).

The RSTOIC block specifies reaction R1 together with the target fractional conversion of the limiting reagent (80%) and computes the resulting product distribution and reactor duty without requiring reaction-rate (kinetic) expressions; it is, by design, an equilibrium/target-conversion representation rather than a rate-based reactor model, and its outputs should be interpreted accordingly (see Limitations). The FLASH2 block performs a rigorous two-phase vapour–liquid flash calculation at the specified temperature and pressure, using the NRTL/ideal-gas thermodynamic framework described in Section 2.1 to split the reactor effluent into a vapour stream (acetylene-rich) and a liquid stream (product- and DMSO-rich). For the RSTOIC reactor, temperature and pressure were set to 90 °C and 1.52 bar, respectively, with a predominant liquid phase characterised by a low outlet vapour-phase fraction (Vapf = 0.028). Calculated heat duty was −0.1133 Gcal·h-1, indicating relatively mild exothermic conditions. The flash separation was performed using a FLASH2 block with the same operating conditions as the RSTOIC reactor. Steady-state conditions, no side reactions, 80% conversion, vapour-phase ideality, and zero-pressure-drop assumptions were used in this simulation. Closure of the overall mass and energy balances was checked as a necessary numerical-consistency test of the simulation (not, by itself, evidence of the model's predictive validity); this check, together with the property-estimation MAE described above, is what is referred to throughout this paper as internal model verification.

## 3. Results and discussion

The results are examined from four complementary perspectives: (i) closure of the mass and energy balances, which is a necessary numerical-consistency condition for the simulation rather than a measure of process performance in itself, (ii) reactor behaviour and product formation, (iii) phase equilibrium, and (iv) the overall thermodynamic and energetic consistency of the reaction, evaluated for the single lumped stoichiometric reaction R1 only (see Section 2.1); the individual mono- and di-vinyl intermediate steps and any side reactions are not separately resolved by this equilibrium-based model. The total mass passing through the system is 1384.82 $kg \cdot h^{-1}$ (**Table 1**), and the balance closes exactly, confirming that the simulation is numerically consistent. However, the molar flow rate decreases from 19.1 to 16.7 $kmol \cdot h^{-1}$ because the reaction converts three molecules of acetylene into one molecule of product. Such behaviour is consistent with the stoichiometric equation under consideration, in which three molecules of acetylene interact with one molecule of the substrate. Total enthalpy of the reaction changes from −0.57841 to −0.69171 $Gcal \cdot h^{-1}$; thus, the heat of reaction equals −0.1133 $Gcal \cdot h^{-1}$.

**Table 1.** Integrated mass and energy balance results for the vinylation process.

| Parameter | Inlet | Outlet | Change |
|---|---|---|---|
| Total molar flow rate ($kmol \cdot h^{-1}$) | 19.1 | 16.7 | -2.4 |
| Total mass flow rate ($kg \cdot h^{-1}$) | 1384.82 | 1384.82 | ≈0 |
| Enthalpy ($Gcal \cdot h^{-1}$) | -0.57841 | -0.69171 | -0.1133 |
| $C_3H_3N_3O_3$ (substrate) ($kmol \cdot h^{-1}$) | 1.0 | 0.2 | -0.8 |
| $C_2H_2$ (acetylene) ($kmol \cdot h^{-1}$) | 3.0 | 0.6 | -2.4 |
| DMSO (solvent) ($kmol \cdot h^{-1}$) | 15.0 | 15.0 | 0 |
| KOH (catalyst) ($kmol \cdot h^{-1}$) | 0.1 | 0.1 | 0 |
| $C_9H_9N_3O_3$ (product) ($kmol \cdot h^{-1}$) | 0.0 | 0.8 | 0.8 |

Concerning the designated conversion level of 80% (90 °C and 1.52 bar), the cyanuric acid substrate transforms 0.8 $kmol \cdot h^{-1}$ of trivinyl compound $C_9H_9N_3O_3$, with a drop in acetylene rate from 3.0 to 0.6 $kmol \cdot h^{-1}$, which is consistent with the stoichiometric proportion. The non-reactivity of DMSO and KOH under these conditions is a direct consequence of the reaction stoichiometry specified in the RSTOIC block. It is reported here for completeness rather than as an independent finding.

The low vapour rate at the reactor outlet (0.028) further supports the predominantly liquid-phase operation. The important reaction and operation data are provided in **Table 2**. Because reaction R1 lumps all vinylation steps into a single net transformation, the model, by construction, does not predict a distribution of mono-, di- and tri-vinyl products; possible formation of these intermediates, and of any other secondary products, is therefore not assessed by the present simulation and should be treated as an open question for future kinetic and analytical (e.g., chromatographic) work.

**Table 2.** Reaction stoichiometry and key reactor operating parameters.

| Category | Parameter | Value |
|---|---|---|
| Reaction Stoichiometry | $C_3H_3N_3O_3$ stoichiometric coefficient | -1.0 |
| | $C_2H_2$ stoichiometric coefficient | -3.0 |
| | $C_9H_9N_3O_3$ stoichiometric coefficient | +1.0 |
| Reactor Conditions | Temperature (°C) | 90.0 |
| | Pressure (bar) | 1.52 |
| | Heat duty ($Gcal \cdot h^{-1}$) | -0.1133 |
| | Vapor fraction | 0.028 |
| | Conversion | 80% |
| | Reaction extent ($kmol \cdot h^{-1}$) | 0.8 |

The phase analysis shows that the reactor outlet consists mainly of liquids, with a liquid fraction of 0.9721. This means there will be no difficulty with mass-transfer resistance downstream of the reactor, thereby allowing proper contact between components in the separation train. After the reaction, the flash separator separates the mixture: the liquid effluent stream, containing a liquid fraction of about 0.9999, consists mostly of trivinylated product and DMSO, and the vapour effluent stream, containing a vapour fraction of 0.9904, consists of acetylene. **Table 3** summarises the temperature, pressure, phase fraction, enthalpy, and density of every stream in the flowsheet. The mixed-feed stream leaves the MIXER at 58.17 °C and 2.03 bar; these values are not independently specified but result from the adiabatic mixing (mass- and energy-weighted flash equilibrium) of the two feed streams at their respective inlet conditions, computed automatically by the MIXER block. The combined stream is then brought to the RSTOIC block's specified operating point (90 °C, 1.52 bar) inside the reactor block itself. Readers seeking to reproduce this step should note that the exact mixed-feed condition depends on the individual FEED1/FEED2 inlet temperatures and pressures specified upstream of the MIXER block.

**Table 3.** Stream characteristics and phase distribution across process units.

| Stream | Gas frac. | Liquid frac. | T (°C) | P (bar) | Enthalpy ($Gcal \cdot h^{-1}$) | Density ($kg \cdot m^3$) |
|---|---|---|---|---|---|---|
| Mixed feed | 0.140 | 0.860 | 58.17 | 2.03 | -0.578 | 37.02 |
| Feed (liquid) | 0.000 | 1.000 | – | – | -0.742 | 1151.56 |
| Feed (gas) | 1.000 | 0.000 | – | – | 0.164 | 2.09 |
| Reactor outlet | 0.028 | 0.972 | 90.0 | 1.52 | -0.692 | 131.78 |
| Product stream | 0.000 | 1.000 | 90.0 | 1.52 | -0.717 | 1090.46 |
| Off-gas stream | 1.000 | 0.000 | 90.0 | 1.52 | 0.025 | 1.36 |
| Mixed feed | 0.140 | 0.860 | 58.17 | 2.03 | -0.578 | 37.02 |

VLE analysis (**Table 4**) provides a thermodynamic foundation for the process under discussion. Acetylene has a very high K value, approximately 111 (K>1), due to its low boiling point of -84 °C at 1 atm, making it volatile[20]. On the other hand, the product of interest has a K of $7.54*10^{-5}$, and DMSO has a K of $2.09*10^{-2}$; both are mainly present in the liquid state, while KOH can be considered non-volatile (K=0). The considerable difference in volatility facilitates separating the product from acetylene via a simple flash step, avoiding the need for additional separation stages; off-gas acetylene recycling should nonetheless be considered for industrial applications to improve raw material utilisation.

**Table 4.** Vapour-liquid equilibrium analysis: component distribution and K-values at flash conditions (90 °C, 1.52 bar).

| Component | $z_i$ (overall) | $x_i$ (liquid) | $y_i$ (vapour) | $K_i = y_i/x_i$ | Phase behavior |
|---|---|---|---|---|---|
| $C_3H_3N_3O_3$ | 0.01198 | 0.01232 | $5.12*10^{-6}$ | $4.16*10^{-4}$ | Non-volatile (liquid phase) |
| $C_2H_2$ | 0.03593 | 0.00883 | 0.98066 | $1.11*10^{2}$ | Highly volatile (vapour phase) |
| DMSO | 0.89820 | 0.92341 | 0.01934 | $2.09*10^{-2}$ | Strong liquid retention |
| KOH | 0.00599 | 0.00616 | 0.00000 | ≈0 | Non-volatile (liquid phase) |
| $C_9H_9N_3O_3$ | 0.04790 | 0.04928 | $3.72*10^{-7}$ | $7.54*10^{-5}$ | Heavy product (liquid phase) |

Thermophysical properties calculated using the Joback group-contribution method yield critical parameters Tc = 902.05 K, Pc = $3.45*10^6$ Pa, Vc = 0.5755 $m^3 \cdot kmol^{-1}$, and Zc = 0.2646, along with an acentric factor of 0.8088. These values are physically plausible for the investigated bulky, polar, heterocyclic nitrogenous compound: the acentric factor and Zc fall within the ranges typically reported for structurally similar multi-substituted heterocycles, and the estimated critical temperature and pressure obey the expected corresponding-states trends relative to related, smaller triazine derivatives; this is what is meant by 'internal consistency in this context. DIPPR-based property estimates (**Table 5**) show mean absolute deviations (MAE) of no more than 2% when benchmarked against Aspen's internal reference database, with thermal conductivity (0.172%) and surface tension (0.0%) being the most accurate predictions. The largest deviation is observed in liquid viscosity prediction (1.73%–1.728%, **Table 5**), which can be considered satisfactory given the intrinsic difficulty of predicting the viscosity of heavy polar compounds using group-contribution methods. As noted in Section 2.1, no independent experimental measurement exists for the specific trivinyl cyanurate product, so these MAE values reflect internal Aspen benchmarking against structurally related compounds rather than a direct experimental validation of this exact molecule.

**Table 5.** Thermophysical properties of $C_9H_9N_3O_3$ and group contribution model validation.

| Property | Value | Unit | Method | MAE (%) | Max Error (%) | Reliability |
|---|---|---|---|---|---|---|
| Heat of vaporisation | — | — | DIPPR | 0.962 | 2.26 | High |
| Molar volume | — | — | DIPPR | 1.445 | 4.12 | Acceptable |
| Vapor viscosity | — | — | DIPPR | 0.519 | 1.08 | High |
| Liquid viscosity | — | — | DIPPR | 1.728 | 3.25 | Acceptable |
| Thermal conductivity | — | — | DIPPR | 0.172 | 0.54 | Very high |
| Surface tension | — | — | DIPPR | 0.0 | 0.0 | Excellent |

Because no directly comparable Aspen-based flowsheet simulation of this reaction exists in the open literature (Section 1), a quantitative benchmark against an equivalent simulation study is not possible; this absence of a direct simulation counterpart is itself part of the gap this work addresses. Qualitatively, the simulated 80% cyanuric-acid conversion and mild exothermic heat duty are consistent with the operating regime reported for the experimental, laboratory-scale KOH/DMSO-catalysed synthesis of vinyl esters of cyanuric acid, for which the present conversion target and operating temperature/pressure were selected (Section 2.1); the process methodology itself (steady-state Aspen Plus flowsheet with NRTL non-ideality and group-contribution property estimation) follows precedents established for other strongly non-ideal, industrially relevant liquid systems such as amine-based $CO_2$ absorption and ionic-liquid processes. A rigorous, quantitative comparison of conversion, thermal load, and separation efficiency against the cited experimental studies would require kinetic and compositional data (e.g., measured yields of mono-, di-, and tri-vinyl products) that are not reported in those sources in a directly comparable form, and is therefore identified as a priority for future work rather than attempted here.

Overall, these findings suggest that the new process operates within physically sound and practical conditions. The difference in volatility between acetylene and the product-solvent pair enables straightforward downstream separation of the product stream via a single flash step. It should be emphasised, however, that the reacting system is intrinsically multiphase (gaseous acetylene reacting with dissolved cyanuric acid in the liquid DMSO/KOH phase); the true reaction rate in practice will be governed by gas–liquid mass transfer across this interface, which is not represented by the equilibrium/target-conversion RSTOIC formulation used here. Adequate gas-liquid contacting (e.g., a well-mixed autoclave or gas-sparged reactor) would therefore be required in an actual reactor design, and this mass-transfer dimension is identified as an important extension for future kinetic and reactor-hydrodynamic modelling, rather than a solved aspect of the current equilibrium-based study. Since the process is generally exothermic, efficient heat removal would be necessary when processing larger amounts of material. At the same time, off-gas acetylene recycling would be an option worth considering for industrial applications.

### 3.1. Limitations

The present model is a preliminary, equilibrium-based screening tool, and its results should be interpreted within the following explicit limitations:

(i) Reactor model: the RSTOIC block enforces a specified (80%) conversion of a single lumped stoichiometric reaction (R1) and contains no reaction-rate (kinetic) expression; it therefore cannot predict how conversion would vary with residence time, mixing intensity, or gas-liquid mass-transfer limitations, and should not be interpreted as a reactor-design or scale-up tool by itself; it is a mass/energy/phase-equilibrium bookkeeping exercise conditioned on an assumed conversion.

(ii) Reaction network: only the overall (fully vinylated) transformation is modelled; the mono- and di-vinyl intermediate species and any side reactions are not tracked individually, so the model cannot report a product distribution or selectivity.

(iii) Thermodynamic model: default (non-regressed) NRTL binary parameters were used in the absence of experimental VLE data for this specific quaternary system, and the conventional molecular NRTL model (rather than the electrolyte-specific ELECNRTL model) was used to represent the KOH-containing liquid phase; both choices introduce quantitative uncertainty in the predicted K-values, although the qualitative phase-distribution trends are expected to remain valid.

(iv) Property estimation: the Joback group-contribution method, while consistent with Aspen Plus defaults and adequate for a preliminary screening study, is known to be less accurate for small molecules; methods such as Marrero–Gani or Ambrose could improve accuracy for the target product and are recommended for future refinement.

(v) Validation basis: no direct experimental (flowsheet-level) validation was available; property MAE values are based on Aspen's internal benchmarking against structurally related compounds rather than direct measurement of the trivinyl cyanurate product itself, and the operating conditions were anchored to literature synthesis conditions rather than to a matched, quantitatively comparable simulation study.

(vi) Gas-liquid mass transfer: the intrinsically multiphase nature of the reacting system (gaseous acetylene / liquid substrate–solvent) means that interfacial mass transfer, not represented in the current equilibrium-based reactor model, is likely to govern the real reaction rate and should be incorporated in future reactor-hydrodynamic and kinetic studies.

Future research efforts must focus on: (i) experimental determination of the kinetic data; (ii) consideration of kinetic and gas-liquid mass-transfer reactor models; (iii) analysis of temperature-pressure-charge composition sensitivity and optimisation; (iv) experimental verification of VLE predictions and

thermophysical properties; and (v) regression of NRTL/ELECNRTL binary interaction parameters against dedicated experimental VLE measurements for the DMSO–acetylene–cyanurate–KOH system.

## 4. Conclusion

In this study, the process of cyanuric acid vinylation by acetylene was thoroughly analysed and modelled using a holistic, physically sound approach within the Aspen Plus framework, explicitly positioned as a preliminary process-screening study rather than a kinetically validated design basis. In this context, considering the reaction stoichiometry, mass and energy balances, the phase behaviour of the reacting system, and estimating VLE data and thermophysical properties within a unified framework enables an accurate description of this chemical process.

The most important results are summarised below:

(i) Mass is conserved in the system at 1384.82 $kg \cdot h^{-1}$; the exothermic process proceeds with an energy release rate of −0.1133 $Gcal \cdot h^{-1}$, confirming that the balances close and that the process is thermodynamically consistent with the specified reaction.

(ii) Under the given operating conditions (T=90℃, P=1.52 bar, target conversion 80%), 0.8 kmol $h^{-1}$ of the desired product is produced in accordance with the experimentally synthesised stoichiometry.

(iii) The reactor operates mostly within a liquid-phase domain (liquid-phase fraction ≈ 0.97), simplifying downstream handling but implying that gas-liquid mass transfer, not represented in the present model, is likely to be rate-controlling in practice (Section 3.1).

(iv) VLE analysis shows that the difference between the components' volatilities is significant: acetylene has a much higher affinity for the vapour phase (K = 111). At the same time, the product and DMSO remain in the liquid phase, meaning phase-based separation is feasible in principle. The group-contribution method yields an MAE of less than 1.73% relative to Aspen's internal reference database (Section 2.1).

(v) The main limitations of the present study, absence of reaction kinetics, use of default NRTL parameters and the conventional (non-electrolyte) NRTL model, and reliance on the Joback group-contribution method are stated explicitly in Section 3.1 and define the priorities for follow-up experimental and modelling work.

In general, this process configuration represents an initial, internally consistent platform for continuous operation and further process engineering development, to be strengthened by future kinetic, mass-transfer, and experimental validation studies.

## Author contributions

Anvar Ziyadullayev: Conceptualization, methodology, investigation, writing- original draft; Bakhodir Abdullayev: Visualization, project administration, writing-reviewing and editing; Odiljon Ziyadullaev: Supervision, visualization, project administration, writing-reviewing and editing, reformatting, grammar editing; Khakimova Guzal, Bunyod Xoliqulov, Fazliddin Xudoyberdiyev, Shavkat Shirinov, Sevara Khakimova, Feruza Karimova, Fozil Juraboyev, Suvonqul Nurmanov, Kamola Ziyadullayeva: Investigation and resource.

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## Conflict of interest

The authors declare no conflict of interest.

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